SGTE DATA FOR PURE ELEMENTS

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ABSTRACT

Thermodynamic data for the condensed phases of 78 elements as currently used by SGTE (Scientific Group Thermodata Europe) are tabulated. SGTE is a consortium of twelve organisations, mainly in Western Europe, engaged in the compilation of a comprehensive, self-consistent and authoritative thermochemical database for inorganic and metallurgical systems. These data are a revision of an earlier publication (91din) which has been used throughout the world as the foundation for the critical assessment of thermodynamic data for binary, ternary and quaternary systems and ultimately of commercial databases for use in modelling materials properties and industrial processes. Since this publication it has been necessary to modify data for some phases of elements in the light of experience and recent experimental work and to extend the range of phases covered for a number of elements. This new publication supercedes this earlier publication.

The data for each phase of each element considered are presented as expressions showing, as a function of temperature, the variation of (a) G-HSER, the Gibbs energy relative to the enthalpy of the "Standard Element Reference" ie the reference phase for the element at 298.15 K and, where appropriate, 1 Pa, and (b) the difference in Gibbs energy between each phase and this reference phase (ie lattice stability). The variation of the heat capacity of the various phases and the Gibbs energy difference between phases are also shown graphically. For certain elements the thermodynamic data have been assessed as a function of pressure as well as temperature. Where appropriate a temperature - pressure phase diagram is also shown.

Throughout this paper the thermodynamic data are expressed in terms of J mol^{-1}. The temperatures of transition between phases have been assessed to be consistent with the 1990 International Temperature Scale (ITS-90).

INTRODUCTION

In this paper the thermodynamic data for the pure elements used by SGTE (Scientific Group Thermodata Europe) are tabulated. SGTE is a consortium of twelve organisations mainly in Western Europe (SIMAP Grenoble, Association THERMODATA, Arcelor Research, RWTH Aachen, KTH Stockholm, NPL, ThermoCalc Software AB, GTT Technologies, Max-Planck-Institut für Metallforschung, Forschungszentrum Jülich, The Spencer Group and ThermFact) engaged in the compilation of a comprehensive, self consistent and authoritative thermochemical database for inorganic and metallurgical systems (86din, 87ans/sun). The main purpose of the database lies in its use in the calculation of phase equilibria in multicomponent systems which puts a premium on the interconsistency of the data and thereby on their traceability to the data for the elements. The SGTE element data were first published in September 1989 (89din) and then modified to conform to the 1990 International Temperature Scale (90pre, 91rus/hud) leading to publication in the CALPHAD journal (91din). Since then these element data have formed the basis of a number of assessments of binary, ternary and higher order systems which have appeared in the open literature. They have as a result formed the basis for a number of commercial databases used for the modelling of materials properties and industrial processes. As a result of new assessment work and experience during assessments this set of data has undergone a series of revisions and enhancements. This paper provides, to the best knowledge of the author, the data for the elements which are currently being used and, indeed, are recommended as the basis of any new critically assessed datasets.

It should be emphasised that these data represent the data that are being used currently. It will soon be necessary to develop a completely new generation of data for the elements based on the latest experimental data, the results of ab-initio calculations and incorporating more physically based models for the extrapolation of data for phases outside the temperature range where they are stable. This was one subject of a series of workshop held at Ringberg (95cha/ans, 95agr/che). The recommendations were far reaching and have still to be implemented.

Stable and Metastable Phase Data

For a given element data are required for each phase in which it can form or dissolve in either in a stable or a metastable state. The data for the stable phases are, on the whole, well defined although serious anomalies still exist requiring further experimental study. Much more of a problem is encountered when one extrapolates the thermodynamic data from a region of temperature in which a given phase is stable to one in which it is metastable. The traditional CALPHAD approach (70kau/ber) is to use the enthalpy and entropy of transition to extrapolate the Gibbs energy difference but to neglect any effects due to a difference in heat capacity between the phases. These differences can often be substantial.

The extrapolation of the experimental heat capacity data across a solid state transformation is generally fairly straightforward. The extrapolation of data above and below the fusion temperature is more complicated. If the liquid heat capacity data are extrapolated from above the fusion temperature to lower temperatures there is the possibility that for certain temperatures the liquid phase would have a lower entropy than the solid phases. This is unreasonable and would be prevented in practice by the occurrence of the so called glass transition, which is thought to take place at between 0.5 and 0.75 of the fusion temperature. A similar problem could occur with the extrapolation of the solid phase data to temperatures well above the melting point where under certain circumstances the solid could be predicted to become stable again.

These problems need to be avoided and SGTE has adopted an interim solution for many elements in which the heat capacity of the liquid phase approaches that of the most stable solid phase for temperatures below the melting point (87and/fer1). In a similar way above the melting temperature the heat capacity of the solid phases approaches that of the liquid phase. This has led to the introduction of terms in T^7 and T^{-9} into expressions for the Gibbs energy and removes the possibility of phases becoming incorrectly stable at high or low temperatures. More recently an alternative method has been used for a number of elements which obtains a smoother extrapolation of the heat capacities of the solid and liquid phases.

Data for phases which, for a given element, are metastable present more of a problem and it has been common to assess these "lattice stabilities", ie expressions for the difference in Gibbs energy between one phase and another, from the critical assessment of data for many binary systems. Many of the lattice stabilities used originally were derived by Kaufman (see for example 70kau/ber, 77kau, 78kau). More recently attempts have been made to define new values for the Gibbs energies of transformation (86sau/mio, 88sau/mio) by considering more recent experimental data for stable phase transformations, taking account of the observed correlation between the entropy of fusion and temperature of fusion and better theoretical prediction of the enthalpy difference between two structures for a given element at 0 K. The findings have also been questioned for some elements (87and/fer2, 87fer/hil). The data given in this document provide, according to the consensus of SGTE members the most reliable data for the elements. The recommended data may change in the course of time as new information becomes available from experimental studies and improved theoretical methods. It should be pointed out that data for the liquid phases of nitrogen and oxygen relative to the gas phase do not reflect real molecular liquids of these elements. The data listed here had been selected as best representing the thermodynamic properties of metal-nitrogen and metal-oxygen systems at high temperatures and for metal rich compositions. In addition data for BCC_A2, HCP_A3 and FCC_A1 phases of B are included in the compilation for completeness although it is currently recommended that B be modelled as dissolving interstitially in these phases.

Standard Element Reference

The data for each phase are stored in the form of Gibbs energies relative to the "Standard Element Reference" ie the enthalpies of the pure elements in their defined reference phase at 298.15 K (denoted as G-HSER). This reference phase is normally the phase stable at 100 kPa and 298.15 K. The exception to this rule is phosphorus for which, by convention, the white form is chosen as the reference phase because the more stable red form is difficult to characterise. This form of data is very convenient to use since all data in a database stored relative to this reference state are interconsistent and can be combined for the calculation of chemical and metallurgical equilibria. Furthermore each dataset contains all the thermodynamic information of interest for a particular phase and does not include any anomalous behaviour in a reference phase. All other thermodynamic functions can be calculated directly from one or more derivatives of the Gibbs energy expression. The concept of G-HSER can be best understood by noting that a Gibbs energy can be subdivided into its enthalpy and entropy contributions. The entropy of an element in a phase has an absolute value. The enthalpy, on the other hand, and therefore the Gibbs energy, has no absolute value, and a reference state needs to be defined. The most obvious reference state for the enthalpy is that of the element in its reference phase at 298.15 K. This is the reference state used for tabulation of the enthalpy of formation at 298.15 K. Combination of the enthalpy defined in this way with the absolute entropy gives G-HSER. This method of expressing Gibbs energy is also used in the Barin and Knacke tables (73bar/kna, 77bar/kna).

Representation of data for the elements

The Gibbs energy is represented as a power series in terms of temperature T in the form:

$$G = a + b\,T + c\,T\,\ln(T) + \sum d\,T^{n}$$

where a, b, c and d are coefficients and n represents a set of integers, typically taking the values of 2, 3 and -1. A number of such expressions are usually required for a given phase to cover the whole temperature range of interest. From this expression for the Gibbs energy other thermodynamic functions can be evaluated:

$$S = -b - c - c\ln(T) - \sum n\,d\,T^{n-1}$$
$$H = a - c\,T - \sum (n-1)\,d\,T^{n}$$
$$Cp = -c - \sum n\,(n-1)\,d\,T^{n-1}$$

In some cases additional terms have been added to the expression for the Gibbs energy in the form of a pressure dependent contribution (Gpres) or a magnetic contribution (Gmag). The pressure dependence for condensed phases is expressed in the form of the Murnaghan equation (44mur, 85fer/gus)

$$Gpres = \frac{A \exp(a_0 T + a_1 T^2/2 + a_2 T^3/3 + a_3 T^{-1})}{(K_0 + K_1 T + K_2 T^2)(n-1)} \; [1 + nP(K_0 + K_1 T + K_2 T^2))^{1-1/n} - 1]$$

where A, a_0, a_1, a_2, a_3, K_0, K_1, K_2 and n are constants for the particular element and phase and P is the pressure. From the well known relationships:

$$V = \left(\frac{\partial G}{\partial P}\right)_T \qquad \alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P \qquad \kappa = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T$$

where V is the molar volume, α is the expansivity and κ is the compressibility. It can be seen from the above equation that the parameter A is equivalent to the molar volume of the material at a temperature of 0 K and a pressure of 0 Pa. Furthermore the parameters a_0, a_1, a_2 and a_3 represent the thermal expansivity of the material as a function of temperature for a pressure of 0 Pa. In an equivalent way the parameters K_0, K_1 and K_2 represent the variation of the compressibility with temperature at zero pressure.

For typical values of K_0, K_1 and K_2 and a value of P of the order of 10^5 Pa or smaller, the expression can be simplified to give:

$$Gpres = AP(1 + a_0 T + a_1 T^2/2 + a_2 T^3/3 + a_3 T^{-1})$$

The contributions to the enthalpy, entropy and heat capacity can also be defined:

$$S_{pres} = -AP(a_0 + a_1 T + a_2 T^2 - a_3 T^{-2})$$

$$H_{pres} = AP(1 - a_1 T^2/2 - 2 a_2 T^3/3 + 2 a_3 T^{-1})$$

$$Cp_{pres} = -AP(a_1 T + 2 a_2 T^2 + 2 a_3 T^{-2})$$

For applications relating to low or moderate pressures the contribution from the pressure dependence can be ignored.

The magnetic contribution to the thermodynamic properties has been defined by Hillert and Jarl (78hil/jar) following the work of Inden (76ind, 81ind). According to Hillert and Jarl the contribution to the Gibbs energy is given by:

$$G_{mag} = R\,T \ln(B_0 + 1)\, g(\tau)$$

where τ is T/T*, T* the critical temperature (the Curie temperature T_C for ferromagnetic materials or the Neel temperature T_N for antiferromagnetic materials) and B_0 the average magnetic moment per atom. g(τ) is given by:

$$g(\tau) = 1 - \left[\frac{79\,\tau^{-1}}{140\,p} + \frac{474}{497}\left(\frac{1}{p} - 1\right)\left(\frac{\tau^3}{6} + \frac{\tau^9}{135} + \frac{\tau^{15}}{600}\right) \right] / D \ldots\ldots\ldots\ldots\ \tau \le 1$$

$$g(\tau) = -\left[\frac{\tau^{-5}}{10} + \frac{\tau^{-15}}{315} + \frac{\tau^{-25}}{1500} \right] / D \ldots\ldots\ldots\ldots\ldots\ \tau > 1$$

$$\text{where} \quad D = \frac{518}{1125} + \frac{11692}{15975}\left(\frac{1}{p} - 1\right)$$

The value of p, which can be thought of as the fraction of the magnetic enthalpy absorbed above the critical temperature, depends on the structure. For the simple BCC_A2 phase p = 0.40 (ie D = 1.55828482) while for other common phases encountered p = 0.28 (ie D = 2.342456517).

In a similar way the magnetic contribution to the other thermodynamic properties can be defined.

$$S_{mag} = - R \ln(B_0 + 1)\, f(\tau)$$

$$\text{where} \quad f(\tau) = 1 - \left[\frac{474}{497}\left(\frac{1}{p} - 1\right)\left(\frac{2\tau^3}{3} + \frac{2\tau^9}{27} + \frac{2\tau^{15}}{75}\right) \right] / \text{D} \ldots\ldots\ldots\ \tau \le 1$$

$$f(\tau) = \left[\frac{2\tau^{-5}}{5} + \frac{2\tau^{-15}}{45} + \frac{2\tau^{-25}}{125} \right] / D \ldots\ldots\ldots\ldots\ldots\ \tau > 1$$

$$H_{mag} = R\,T \ln(B_0 + 1)\, h(\tau)$$

$$\text{where} \quad h(\tau) = \left[-\frac{79\,\tau^{-1}}{140\,p} + \frac{474}{497}\left(\frac{1}{p} - 1\right)\left(\frac{\tau^3}{2} + \frac{\tau^9}{15} + \frac{\tau^{15}}{40}\right) \right] / \text{D} \ldots\ldots\ldots\ldots\ \tau \le 1$$

$$h(\tau) = -\left[\frac{\tau^{-5}}{2} + \frac{\tau^{-15}}{21} + \frac{\tau^{-25}}{60}\right] / D \ldots\ldots\ldots\ldots\ldots\ldots \tau > 1$$

$$Cp_{mag} = R \ln(B_0 + 1)\, c(\tau)$$

where $$c(\tau) = \left[\frac{474}{497}\left(\frac{1}{p} - 1\right)\left(2\tau^{3} + \frac{2\tau^{9}}{3} + \frac{2\tau^{15}}{5}\right)\right] / D \ldots\ldots\ldots\ldots\ldots\ldots \tau \leq 1$$

$$c(\tau) = \left[2\tau^{-5} + \frac{2\tau^{-15}}{3} + \frac{2\tau^{-25}}{5}\right] / D \ldots\ldots\ldots\ldots\ldots\ldots \tau > 1$$

The remainder of this document falls into two parts. The first part is a summary of the transition data between the stable phases for all elements for which SGTE has solid and liquid data. All thermodynamic data refer to units of J mol^{-1}. This is similar to the information presented in the Massalski compilation of binary alloy phase diagrams (91din). In this present paper the standard entropies at 298.15 K for certain key elements have been modified to be compatible with the CODATA key values (89cox/wag). Furthermore all temperatures quoted refer to the ITS-90 temperature scale (90pre, 91rus/hud). These include eight of the fixed points on the temperature scale. The temperatures of transition or fusion for a number of other elements have also been modified from the earlier compilation (89din) where the appropriate quantity is known sufficiently accurately. This covers a further 16 elements, some of which were secondary reference points of the IPTS-68 temperature scale. It is felt that transition temperatures for the other elements are not known sufficiently accurately to justify modification (ie the requisite change was significantly smaller than the uncertainty in the measured value).

The second part is a list, for each element, of the data firstly in the form of G-HSER and secondly relative to the element reference phase. For every element the reference phase is the first phase for which data are given. References are provided to the source of the data used. The references most widely quoted ie Hultgren (73hul/des), Saunders et al. (88sau/mio), Kaufman (70kau), TPIS (78gur/vei), CODATA (87gar/pre) and JANAF (85cha/dav) are simply referenced by name. Graphs generated by MTDATA (NPL Software for Thermodynamics and Phase Equilibria) (90dav/din, 02dav/din) are provided to show the variation of heat capacity of the various phases as a function of temperature and also the difference in Gibbs energy between a given phase and the element reference phase. For certain elements the thermodynamic data have been assessed both as a function of temperature and pressure. Where appropriate a temperature - pressure phase diagram is also shown.

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Acknowledgements

The data presented in this paper could not have been compiled without the invaluable help of colleagues at NPL and within SGTE. In particular the author would like to thank M H Rand, formerly of AEA Technology, Harwell for his advice and contributions of data. Fruitful discussions with J W Arblaster are also gratefully acknowledged. The data provided in this paper are also available in computer readable form (version 4.5 of the SGTE Unary database) and may be downloaded from the SGTE web site (www.sgte.org). This work was part supported by the National Measurement System of the UK Department of Trade and Industry.

SGTE PURE ELEMENT TRANSITION DATA

	Atomic wt	H_{298}-H_0/ J mol^{-1}	S_{298}/ J mol^{-1} K^{-1}	Phase	T_{trans}/ K	$\Delta_{trans}H$/ J mol^{-1}	$\Delta_{trans}S$/ J mol^{-1} K^{-1}	$\Delta_{trans}Cp$ J mol^{-1} K^{-1}
Ag	107.8682	5745.	42.55	FCC_A1	1234.93	11296.80	9.1477	1.5402
Al	26.98154	4540.	28.30	FCC_A1	933.473	10711.04	11.4744	-2.2046
Am	243.	6407.00	55.3960	DHCP	1041.98	870.09	0.8350	-2.7810
				FCC_A1	1350.00	5862.06	4.3422	1.2898
				BCC_A2	1449.00	14393.0	9.9330	2.092
As	74.922	5117.032	35.6895	RHO_A7	1090.00	24442.9	22.4247	0.0
Au	196.9665	6016.592	47.4884	FCC_A1	1337.33	12552.0	9.3859	0.0
B	10.81	1222.0	5.9	BET	2348.00	50200.00	21.3799	0.8362
Ba	137.33	6910.0	62.50	BCC_A2	1000.00	7120.0	7.120	-4.3450
Be	9.01218	1950.0	9.50	HCP_A3	1527.00	6849.0	4.4853	-1.8915
				BCC_A2	1560.00	7895.0	5.0609	-1.2123
Bi	208.9804	6426.624	56.735	RHO_A7	544.55	11296.80	20.7452	0.6522
C	12.011	1054.0	5.7423	HEX_A9	4765.3	117369.0	24.6300	0.0
Ca	40.08	5736.0	41.588	FCC_A1	716.00	928.85	1.2972	-1.2336
				BCC_A2	1115.00	8539.54	7.6588	-8.2257
Cd	112.41	6247.	51.80	HCP_A3	594.219	6192.32	10.4209	0.1666
Ce	140.12	7280.16	69.454	FCC_A1	1000.00	2991.60	2.9916	-0.1337
				BCC_A2	1072.00	5460.12	5.0934	0.0836
Co	58.9332	4765.567	30.0400	HCP_A3	694.99	427.59	0.6153	0.000
				FCC_A1	1768.00	16200.01	9.1629	0.8962
Cr	51.996	4050.0	23.5429	BCC_A2	2180.0	21004.00	9.6349	-10.7118
Cs	132.9054	7711.000	85.23	BCC_A2	301.59	2096.00	6.9498	0.1128
Cu	63.546	5004.	33.15	FCC_A1	1357.77	13263.28	9.7684	1.5391
Dy	162.50	8865.896	74.9559	HCP_A3	1654.15	4591.74	2.7759	4.1866
				BCC_A2	1685.11	11350.52	6.7358	-0.2929
Er	167.26	7392.2912	73.17816	HCP_A3	1802.00	19903.29	11.0451	-4.6468
Eu	151.96	8004.0	80.79304	BCC_A2	1095.00	9213.17	8.4139	-2.9731
Fe	55.847	4489.0	27.2797	BCC_A2	1184.81	1012.86	0.8549	-7.6812
				FCC_A1	1667.47	825.78	0.4952	2.1829
				BCC_A2	1810.94	13806.84	7.6241	4.6526
Ga	69.72	5572.0	40.7271	ORT	302.91	5589.81	18.4534	2.2766
Gd	157.25	9087.648	68.0894	HCP_A3	1508.15	3518.67	2.3331	-0.3127
				BCC_A2	1586.15	9668.04	6.0953	-0.4529
Ge	72.59	4636.	31.09	DIA_A4	1211.40	36944.72	30.4975	-1.1370
Hf	178.49	5845.0	43.56	HCP_A3	2016.00	5860.29	2.9069	-6.6207
				BCC_A2	2506.00	27196.00	10.8524	5.5559

	Atomic wt	H_{298}-H_0	S_{298}	Phase	T_{trans}	$\Delta_{trans}H$	$\Delta_{trans}S$	$\Delta_{trans}Cp$
Hg	200.59	9342.	75.90	LIQUID	234.321	2295.34	9.7957	-0.0066
Ho	164.9304	7995.624	75.0191	HCP_A3	1747.00	15926.61	9.1165	-9.7986
In	114.82	6610.0	57.65	TET_A6	429.7485	3283.0	7.6393	0.0148
Ir	192.22	5267.656	35.5054	FCC_A1	2719.00	41124.00	15.1247	12.0550
K	39.0983	7088.	64.68	BCC_A2	336.53	2320.86	6.8964	0.0576
La	138.9055	6665.112	56.9024	DHCP	550.00	364.01	0.6618	-0.5686
				FCC_A1	1134.00	3121.26	2.7524	4.5150
				BCC_A2	1193.00	6196.50	5.1941	-5.2300
Li	6.941	4632.00	29.12	BCC_A2	453.60	2999.93	6.6136	0.6362
Lu	174.967	6388.968	50.9611	HCP_A3	1936.00	18648.09	9.6323	-0.0103
Mg	24.305	4998.0	32.671	HCP_A3	923.00	8476.78	9.1839	2.0821
Mn	54.9380	4995.696	32.2206	CBCC_A12	980.00	2253.55	2.2995	-1.5482
				CUB_A13	1360.00	2165.73	1.5925	0.1264
				FCC_A1	1411.00	1908.30	1.3524	3.2651
				BCC_A2	1519.00	12908.94	8.4983	1.7204
Mo	95.94	4589.0	28.56	BCC_A2	2896.00	37479.85	12.9419	-10.5181
Na	22.98977	6460.	51.3000	BCC_A2	370.87	2597.01	7.0025	0.3018
Nb	92.9064	5220.0	36.27	BCC_A2	2750.00	30000.0	10.9091	0.5560
Nd	144.24	7133.72	71.0862	DHCP	1128.00	3029.22	2.6855	-1.435
				BCC_A2	1289.00	7142.09	5.5408	4.2258
Ni	58.69	4787.0	29.7955	FCC_A1	1728.30	17479.82	10.1142	4.248
Np	237.0482	6606.536	50.4590	ORTHO	555.02	4699.92	8.4680	-5.0491
				TETRAG	855.95	3000.12	3.5050	-2.9291
				BCC_A2	916.84	3198.57	3.4887	8.995
Os	190.2		32.6352	HCP_A3	3306.00	57855.00	17.5000	13.8379
P	30.97376	5360.0	41.09	WHITE	317.30	659.0	2.0769	1.9793
Pa	231.0359	6439.176	51.882	BCT_Aa	1443.10	6639.79	4.6011	-2.0962
				BCC_A2	1844.78	12341.18	6.6898	7.5305
Pb	207.2	6870.	64.80	FCC_A1	600.612	4773.94	7.9485	1.1867
Pd	106.42	5468.488	37.8234	FCC_A1	1828.00	16736.00	9.1554	4.5325
Pr	140.9077	7418.232	73.9313	DHCP	1068.00	3167.29	2.9656	-3.5564
				BCC_A2	1204.00	6886.86	5.7200	4.5187
Pt	195.08	5723.712	41.6308	FCC_A1	2041.50	22175.00	10.8621	-0.8317
Pu	244.	6902.0	54.4610		397.61	3706.00	9.3206	-3.3379
					487.90	478.00	0.9797	-0.5630
					593.06	713.02	1.2023	-0.7521
				FCC_A1	736.40	83.35	0.1132	-0.8764
				TET_A6	755.67	1841.06	2.4363	-1.8400
				BCC_A2	913.00	2824.03	3.0931	8.4470

	Atomic wt	H_{298}-H_0	S_{298}	Phase	T_{trans}	$\Delta_{trans}H$	$\Delta_{trans}S$	$\Delta_{trans}Cp$
Rb	85.4678	7489.	76.78	BCC_A2	312.46	2192.42	7.0166	-0.5631
Re	186.207	5333.	36.4820	HCP_A3	3458.00	34075.04	9.8540	9.9322
Rh	102.9055	(4920.384)	31.5557	FCC_A1	2237.00	26593.50	11.8880	1.3593
Ru	101.07	4602.4	28.6144	HCP_A3	2607.00	38589.03	14.8021	0.8342
S	32.06	4412.0	32.07	ORTHO	368.30	401.00	1.0888	0.5358
				MONOCL	388.36	1721.00	4.4315	6.5224
Sb	121.75	5870.152	45.5219	RHO_A7	903.78	19874.00	21.9899	0.4002
Sc	44.9559	5217.448	34.6435	HCP_A3	1608.00	4008.27	2.4927	4.1361
				BCC_A2	1814.00	14095.90	7.7706	0.000
Se	78.96	5514.512	41.9655	HEX_A8	494.00	6694.40	13.5514	3.8536
Si	28.0855	3217.	18.81	DIA_A4	1687.00	50208.00	29.7617	-2.0264
Sm	150.36	7573.04	69.4962	RHOMB_C19	1007.00	69.98	0.0695	0
				HCP_A3	1195.00	3035.75	2.5404	-1.4892
				BCC_A2	1345.00	8619.04	6.4082	3.2635
Sn	118.69	6323.	51.18	BCT_A5	505.078	7029.12	13.9169	-1.0252
Sr	87.62	6568.	55.694	FCC_A1	820.00	836.80	1.0205	-2.3609
				BCC_A2	1050.00	7431.00	7.0771	8.7110
Ta	180.9479	5681.872	41.4718	BCC_A2	3290.00	36568.17	11.1149	-2.6340
Tb	158.9254	9426.552	73.3037	HCP_A3	1562.00	4380.65	2.8045	-0.3402
				BCC_A2	1632.00	10150.38	6.2196	0.000
Tc	98.		32.9856	HCP_A3	2430.01	33291.19	13.7000	8.3218
Te	127.60	6080.	49.221	HEX_A8	722.66	17376.00	24.0445	16.1903
Th	232.0381	6350.	51.8	FCC_A1	1633.20	3597.01	2.2024	-5.7949
				BCC_A2	2022.99	13807.13	6.8251	6.0679
Ti	47.88	4824.	30.72	HCP_A3	1155.00	4169.98	3.6104	-5.0307
				BCC_A2	1941.00	14146.00	7.2880	8.4656
Tl	204.383	6831.97	64.2997	HCP_A3	507.00	359.82	0.7097	2.0997
				BCC_A2	577.00	4142.16	7.1788	-2.3901
Tm	168.9342	7397.312	74.01496	HCP_A3	1818.00	16840.60	9.2633	3.8918
U	238.0289	6364.	50.20	ORT_A20	942.00	2790.73	2.9625	-5.111
				TET	1049.00	4757.18	4.5350	-4.644
				BCC_A2	1408.00	9142.04	6.4930	10.3764
V	50.9415	4507.0	30.89	BCC_A2	2183.00	21500.0	9.8488	2.3597
W	183.85	4970.0	32.6176	BCC_A2	3694.90	52313.66	14.1583	0.2900
Y	88.9059	5983.457	44.7875	HCP_A3	1751.15	4886.19	2.7903	-3.5825
				BCC_A2	1795.15	11394.22	6.3472	7.9486
Yb	173.04	6711.136	59.8312	FCC_A1	1033.00	1748.91	1.6930	4.059
				BCC_A2	1097.00	7656.72	6.9797	0.6695
Zn	65.38	5657.	41.63	HCP_A3	692.68	7322.00	10.5705	1.6653
Zr	91.22	5566.27	39.1809	HCP_A3	1138.97	4106.54	3.6054	-6.3115
				BCC_A2	2127.85	20997.77	9.8681	6.0320

Ag

Source of data: *Hultgren [FCC_A1, LIQUID]*
Saunders et al. [HCP_A3, BCC_A2]
S S Lim, P L Rossiter, J W Tibballs; CALPHAD, 1995, 19(2),131-142 [CUB_A13]
C S Oh, J H Shim, B J Lee, D N Lee; J. Alloys Compounds, 1996, 238, 155-66 [BCT_A5]
A T Dinsdale, Unpublished work [HCP_ZN]

FCC_A1

$-7209.512 + 118.202013\,T - 23.8463314\,T\ln(T) - 1.790585E{-3}\,T^2 - 0.398587E{-6}\,T^3 - 12011\,T^{-1}$ *(298.15 < T < 1234.93)*

$-15095.252 + 190.266404\,T - 33.472\,T\ln(T) + 1411.773E26\,T^{-9}$ *(1234.93 < T < 3000)*

LIQUID

$3815.564 + 109.310993\,T - 23.8463314\,T\ln(T) - 1.790585E{-3}\,T^2 - 0.398587E{-6}\,T^3 - 12011\,T^{-1} - 1033.905E{-23}\,T^7$ *(298.15 < T < 1234.93)*

$-3587.111 + 180.964656\,T - 33.472\,T\ln(T)$ *(1234.93 < T < 3000)*

HCP_A3

$-6909.512 + 118.502013\,T - 23.8463314\,T\ln(T) - 1.790585E{-3}\,T^2 - 0.398587E{-6}\,T^3 - 12011\,T^{-1}$ *(298.15 < T < 1234.93)*

$-14795.252 + 190.566404\,T - 33.472\,T\ln(T) + 1411.773E26\,T^{-9}$ *(1234.93 < T < 3000)*

BCC_A2

$-3809.512 + 117.152013\,T - 23.8463314\,T\ln(T) - 1.790585E{-3}\,T^2 - 0.398587E{-6}\,T^3 - 12011\,T^{-1}$ *(298.15 < T < 1234.93)*

$-11695.252 + 189.216404\,T - 33.472\,T\ln(T) + 1411.773E26\,T^{-9}$ *(1234.93 < T < 3000)*

BCT_A5

$-3025.412 + 118.202013\,T - 23.8463314\,T\ln(T) - 1.790585E{-3}\,T^2 - 0.398587E{-6}\,T^3 - 12011\,T^{-1}$ *(298.15 < T < 1234.93)*

$-10911.152 + 190.266404\,T - 33.472\,T\ln(T) + 1411.773E26\,T^{-9}$ *(1234.93 < T < 3000)*

CUB_A13

$-3809.512 + 117.152013\,T - 23.8463314\,T\ln(T) - 1.790585E{-3}\,T^2 - 0.398587E{-6}\,T^3 - 12011\,T^{-1}$ *(298.15 < T < 1234.93)*

$-11695.252 + 189.216404\,T - 33.472\,T\ln(T) + 1411.773E26\,T^{-9}$ *(1234.93 < T < 3000)*

HCP_ZN

$-6809.512 + 118.502013\ T - 23.8463314\ T\ \ln(T) - 1.790585E\text{-}3\ T^{2} - 0.398587E\text{-}6\ T^{3} - 12011\ T^{-1}$ *(298.15 < T < 1234.93)*

$-14695.252 + 190.566404\ T - 33.472\ T\ \ln(T) + 1411.773E26\ T^{-9}$ *(1234.93 < T < 3000)*

Data relative to FCC_A1

LIQUID

$11025.076 - 8.89102\ T - 1033.905E\text{-}23\ T^{7}$ *(298.15 < T < 1234.93)*

$11508.141 - 9.301748\ T - 1411.773E26\ T^{-9}$ *(1234.93 < T < 3000)*

HCP_A3

$300 + 0.3\ T$ *(298.15 < T < 3000)*

BCC_A2

$3400 - 1.05\ T$ *(298.15 < T < 3000)*

BCT_A5

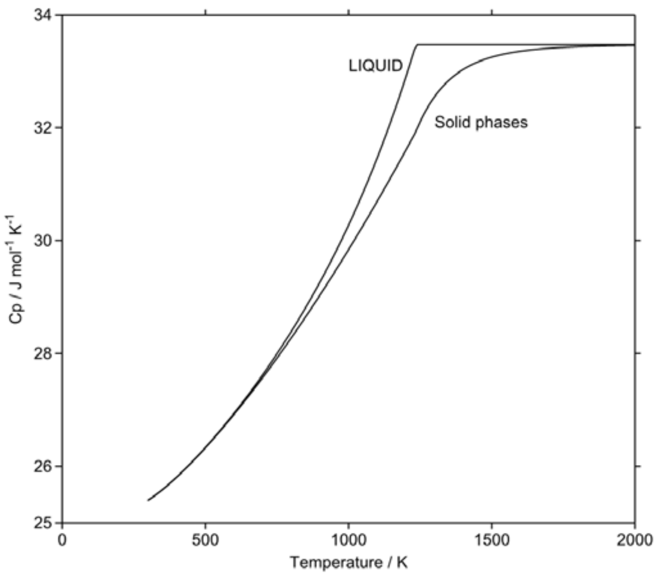
4184.1 *(298.15 < T < 3000)*

CUB_A13

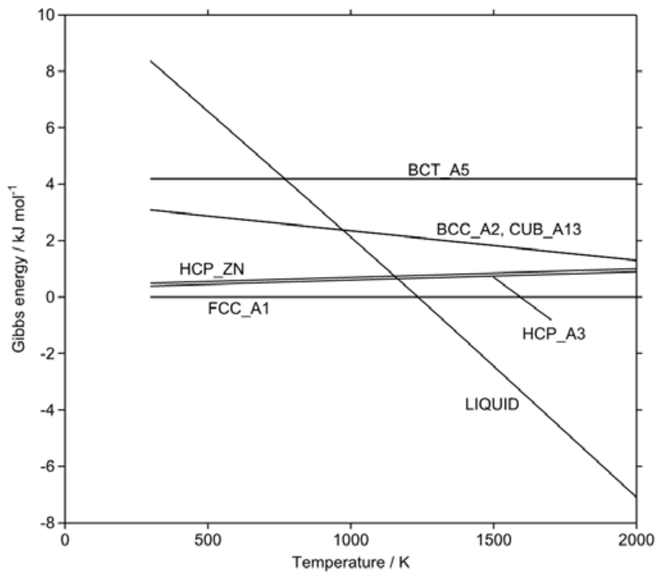
$3400 - 1.05\ T$ *(298.15 < T < 3000)*

HCP_ZN

$400 + 0.3\ T$ *(298.15 < T < 3000)*



Heat capacity of Ag



Gibbs energy of phases of Ag relative to FCC_A1

Al

Source of data: *JANAF [FCC_A1, LIQUID]*
RWTH Aachen, Unpublished work [BCC_A2, BCC_A12]
Kaufman [CUB_A13]
Saunders et al. [HCP_A3]
COST507 database [BCT_A5, DIAMOND_A4]

FCC_A1

$-7976.15 + 137.093038\,T - 24.3671976\,T\ln(T) - 1.884662E\text{-}3\,T^2 - 0.877664E\text{-}6\,T^3 + 74092\,T^{-1}$ *(298.15 < T < 700)*

$-11276.24 + 223.048446\,T - 38.5844296\,T\ln(T) + 18.531982E\text{-}3\,T^2 - 5.764227E\text{-}6\,T^3 + 74092\,T^{-1}$ *(700 < T < 933.473)*

$-11278.361 + 188.684136\,T - 31.748192\,T\ln(T) - 1230.622E25\,T^{-9}$ *(933.473 < T < 2900)*

LIQUID

$3028.895 + 125.251188\,T - 24.3671976\,T\ln(T) - 1.884662E\text{-}3\,T^2 - 0.877664E\text{-}6\,T^3 + 74092\,T^{-1} + 79.34E\text{-}21\,T^7$ *(298.15 < T < 700)*

$-271.194 + 211.206596\,T - 38.5844296\,T\ln(T) + 18.531982E\text{-}3\,T^2 - 5.764227E\text{-}6\,T^3 + 74092\,T^{-1} + 79.34E\text{-}21\,T^7$ *(700 < T < 933.473)*

$-795.991 + 177.430209\,T - 31.748192\,T\ln(T)$ *(933.473 < T < 2900)*

HCP_A3

$-2495.15 + 135.293038\,T - 24.3671976\,T\ln(T) - 1.884662E\text{-}3\,T^2 - 0.877664E\text{-}6\,T^3 + 74092\,T^{-1}$ *(298.15 < T < 700)*

$-5795.24 + 221.248446\,T - 38.5844296\,T\ln(T) + 18.531982E\text{-}3\,T^2 - 5.764227E\text{-}6\,T^3 + 74092\,T^{-1}$ *(700 < T < 933.473)*

$-5797.361 + 186.884136\ T - 31.748192\ T\ ln(T) - 1230.622E25\ T^{-9}$ *(933.473 < T < 2900)*

BCC_A2

$2106.85 + 132.280038\ T - 24.3671976\ T\ ln(T) - 1.884662E\text{-}3\ T^2 - 0.877664E\text{-}6\ T^3 + 74092\ T^{-1}$ *(298.15 < T < 700)*

$-1193.24 + 218.235446\ T - 38.5844296\ T\ ln(T) + 18.531982E\text{-}3\ T^2 - 5.764227E\text{-}6\ T^3 + 74092\ T^{-1}$ *(700 < T < 933.473)*

$-1195.361 + 183.871136\ T - 31.748192\ T\ ln(T) - 1230.622E25\ T^{-9}$ *(933.473 < T < 2900)*

BCT_A5

$2106.85 + 132.280038\ T - 24.3671976\ T\ ln(T) - 1.884662E\text{-}3\ T^2 - 0.877664E\text{-}6\ T^3 + 74092\ T^{-1}$ *(298.15 < T < 700)*

$-1193.24 + 218.235446\ T - 38.5844296\ T\ ln(T) + 18.531982E\text{-}3\ T^2 - 5.764227E\text{-}6\ T^3 + 74092\ T^{-1}$ *(700 < T < 933.473)*

$-1195.361 + 183.871136\ T - 31.748192\ T\ ln(T) - 1230.622E25\ T^{-9}$ *(933.473 < T < 2900)*

DIAMOND_A4

$-7976.15 + 167.093038\ T - 24.3671976\ T\ ln(T) - 1.884662E\text{-}3\ T^2 - 0.877664E\text{-}6\ T^3 + 74092\ T^{-1}$ *(298.15 < T < 700)*

$-11276.24 + 253.048446\ T - 38.5844296\ T\ ln(T) + 18.531982E\text{-}3\ T^2 - 5.764227E\text{-}6\ T^3 + 74092\ T^{-1}$ *(700 < T < 933.473)*

$-11278.361 + 218.684136\ T - 31.748192\ T\ ln(T) - 1230.622E25\ T^{-9}$ *(933.473 < T < 2900)*

CBCC_A12

$2107.25 + 132.280038\ T - 24.3671976\ T\ ln(T) - 1.884662E\text{-}3\ T^2 - 0.877664E\text{-}6\ T^3 + 74092\ T^{-1}$ *(298.15 < T < 700)*

$-1192.84 + 218.235446\ T - 38.5844296\ T\ ln(T) + 18.531982E\text{-}3\ T^2 - 5.764227E\text{-}6\ T^3 + 74092\ T^{-1}$ *(700 < T < 933.473)*

$-1194.961 + 183.871136\ T - 31.748192\ T\ ln(T) - 1230.622E25\ T^{-9}$ *(933.473 < T < 2900)*

CUB_A13

$2944.29 + 132.281438\ T - 24.3671976\ T\ ln(T) - 1.884662E\text{-}3\ T^2 - 0.877664E\text{-}6\ T^3 + 74092\ T^{-1}$ *(298.15 < T < 700)*

$-355.8 + 218.236846\ T - 38.5844296\ T\ ln(T) + 18.531982E\text{-}3\ T^2 - 5.764227E\text{-}6\ T^3 + 74092\ T^{-1}$ *(700 < T < 933.473)*

$-357.921 + 183.872536\ T - 31.748192\ T\ ln(T) - 1230.622E25\ T^{-9}$ *(933.473 < T < 2900)*

HCP_ZN

$-2495.15 + 135.293038\ T - 24.3671976\ T\ ln(T) - 1.884662E\text{-}3\ T^2 - 0.877664E\text{-}6\ T^3 + 74092\ T^{-1}$ *(298.15 < T < 700)*

$-5795.24 + 221.248446\ T - 38.5844296\ T \ln(T) + 18.531982E\text{-}3\ T^2 - 5.764227E\text{-}6\ T^3 + 74092\ T^{-1}$

(700 < T < 933.473)

$-5797.361 + 186.884136\ T - 31.748192\ T \ln(T) - 1230.622E25\ T^{-9}$ *(933.473 < T < 2900)*

Data relative to FCC_A1

LIQUID

$11005.045 - 11.84185\ T + 79.34E\text{-}21\ T^7$ *(298.15 < T < 933.473)*

$10482.37 - 11.253927\ T + 1230.622E25\ T^{-9}$ *(933.473 < T < 2900)*

HCP_A3

5481 - 1.8 T *(298.15 < T < 2900)*

BCC_A2

10083 - 4.813 T *(298.15< T < 2900)*

BCT_A5

10083 - 4.813 T *(298.15< T < 2900)*

DIAMOND_A4

30 T *(298.15 < T < 2900)*

CBCC_A12

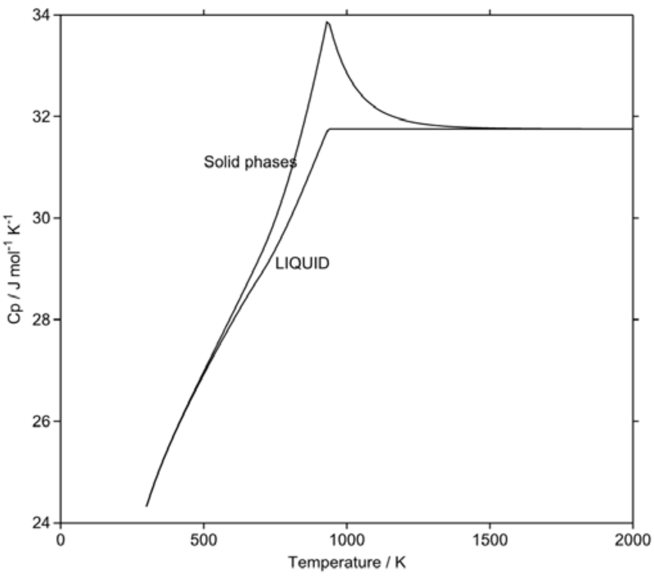
10083.4 - 4.813 T *(298.15 < T < 2900)*

CUB_A13

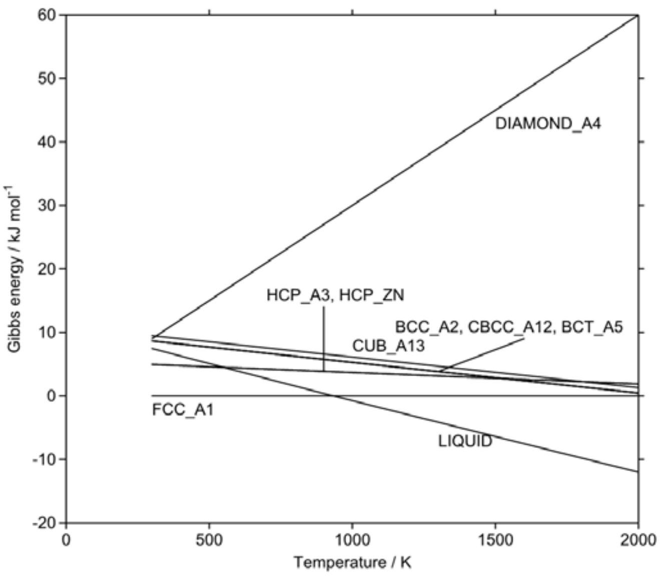
10920.44 - 4.8116 T *(298.15 < T < 2900)*

HCP_ZN

5481 - 1.8 T *(298.15 < T < 2900)*



Heat capacity of Al



Gibbs energy of phases of Al relative to FCC_A1

Am

Source of data: *M H Rand and A T Dinsdale (unpublished work)*

DHCP

$-6639.201 + 89.645685\ T - 21.1868\ T\ln(T) - 5.59955E\text{-}3\ T^2 - 0.541038E\text{-}6\ T^3 - 30424\ T^{-1}$ *(298.15 < T < 1329)*

$-21702.938 + 241.107269\ T - 41.84\ T\ln(T)$ *(1329 < T < 3000)*

LIQUID

$13271.499 + 75.525185\ T - 21.1868\ T\ln(T) - 5.59955E\text{-}3\ T^2 - 0.541038E\text{-}6\ T^3 - 30424\ T^{-1}$ *(298.15 < T < 1329)*

$-1792.238 + 226.986769\ T - 41.84\ T\ln(T)$ *(1329 < T < 3000)*

BCC_A2

$-665.396 + 85.114354\ T - 21.1868\ T\ln(T) - 5.5995E\text{-}3\ T^2 - 0.541033E\text{-}6\ T^3 - 30424\ T^{-1}$ *(298.15 < T < 999)*

$-7800.332 + 63.93115\ T - 15.8832\ T\ln(T) - 19.0671E\text{-}3\ T^2 + 2.291117E\text{-}6\ T^3 + 2287195\ T^{-1}$ *(999 < T < 1339)*

$-13153.887 + 219.600832\ T - 39.748\ T\ln(T)$ *(1339 < T < 1449)*

$70352.138 - 326.394464\ T + 33.413\ T\ln(T) - 27.36485E\text{-}3\ T^2 + 1.801717E\text{-}6\ T^3 - 17379450\ T^{-1}$ *(1449 < T < 2183.6)*

$-16925.244 + 237.367028\ T - 41.84\ T\ln(T)$ *(2183.6 < T < 3000)*

FCC_A1

$-5224.899 + 99.204329\ T - 23.1377\ T \ln(T) - 2.94694E{-3}\ T^2 - 0.664773E{-6}\ T^3 - 18507\ T^{-1}$ *(298.15 < T < 1018)*

$-2935.853 + 73.800069\ T - 19.4406\ T \ln(T) - 5.418E{-3}\ T^2 - 0.375233E{-6}\ T^3 - 260435\ T^{-1}$ *(1018 < T < 1548.7)*

$-22179.593 + 241.353807\ T - 41.84\ T \ln(T)$ *(1548.7 < T < 3000)*

Data relative to DHCP

LIQUID

$19910.7 - 14.1205\ T$ *(298.15 < T < 3000)*

BCC_A2

$5973.805 - 4.531331\ T + 0.00005E{-3}\ T^2 + 0.000005E{-6}\ T^3$ *(298.15 < T < 999)*

$-1161.131 - 25.714535\ T + 5.3036\ T \ln(T) - 13.46755E{-3}\ T^2 + 2.832155E{-6}\ T^3 + 2317619\ T^{-1}$ *(999 < T < 1329)*

$13902.606 - 177.176119\ T + 25.9568\ T \ln(T) - 19.0671E{-3}\ T^2 + 2.291117E{-6}\ T^3 + 2287195\ T^{-1}$ *(1329 < T < 1339)*

$8549.051 - 21.506437\ T + 2.092\ T \ln(T)$ *(1339 < T < 1449)*

$92055.076 - 567.501733\ T + 75.253\ T \ln(T) - 27.36485E{-3}\ T^2 + 1.801717E{-6}\ T^3 - 17379450\ T^{-1}$ *(1449 < T < 2183.6)*

$4777.694 - 3.740241\ T$ *(2183.6 < T < 3000)*

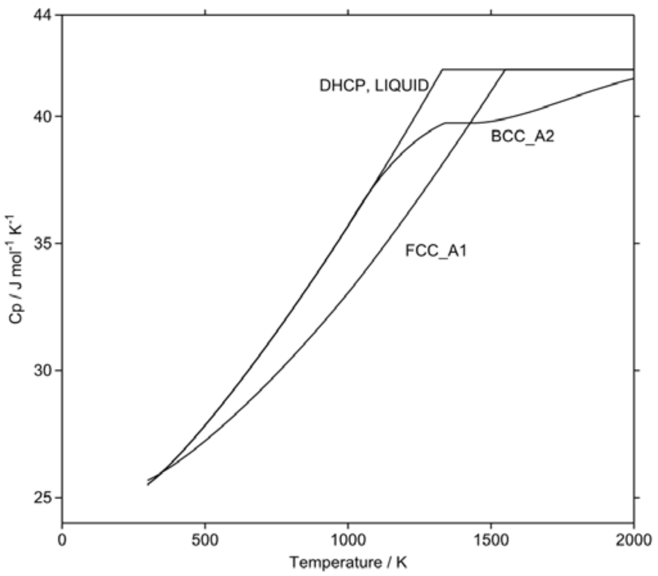
FCC_A1

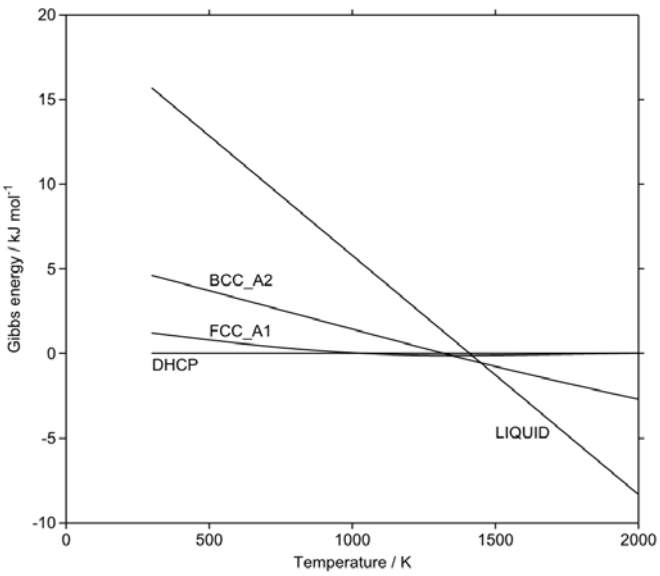
$1414.302 + 9.558644\ T - 1.9509\ T \ln(T) + 2.65261E{-3}\ T^2 - 0.123735E{-6}\ T^3 + 11917\ T^{-1}$ *(298.15 < T < 1018)*

$3703.348 - 15.845616\ T + 1.7462\ T \ln(T) + 0.18155E{-3}\ T^2 + 0.165805E{-6}\ T^3 - 230011\ T^{-1}$ *(1018 < T < 1329)*

$18767.085 - 167.3072\ T + 22.3994\ T \ln(T) - 5.418E{-3}\ T^2 - 0.375233E{-6}\ T^3 - 260435\ T^{-1}$ *(1329 < T < 1548.7)*

$-476.655 + 0.246538\ T$ *(1548.7 < T < 3000)*





Heat capacity of Am

Gibbs energy of phases of Am relative to DHCP

As

Source of data: *Hultgren modified by I Ansara [RHOMBO_A7, LIQUID]*
Saunders et al. [HCP_A3, BCC_A2, FCC_A1]

RHOMBOHEDRAL_A7

-7270.447 + 122.211069 T - 23.3144 T ln(T) - 2.71613E-3 T^2 + 11600 T^{-1} *(298.15 < T < 1090)*
-10454.913 + 163.457433 T - 29.216037 T ln(T) *(1090 < T < 1200)*

LIQUID

17172.453 + 99.78639 T - 23.3144 T ln(T) - 2.71613E-3 T^2 + 11600 T^{-1} *(298.15 < T < 1090)*
13987.987 + 141.032754 T - 29.216037 T ln(T) *(1090 < T < 1200)*

BCC_A2

17603.553 + 106.111069 T - 23.3144 T ln(T) - 2.71613E-3 T^2 + 11600 T^{-1} *(298.15 < T < 1090)*
14419.087 + 147.357433 T - 29.216037 T ln(T) *(1090 < T < 1200)*

FCC_A1

17603.553 + 107.471069 T - 23.3144 T ln(T) - 2.71613E-3 T^2 + 11600 T^{-1} *(298.15 < T < 1090)*
14419.087 + 148.717433 T - 29.216037 T ln(T) *(1090 < T < 1200)*

HCP_A3

17603.553 + 108.211069 T - 23.3144 T ln(T) - 2.71613E-3 T^2 + 11600 T^{-1} *(298.15 < T < 1090)*
14419.087 + 149.457433 T - 29.216037 T ln(T) *(1090 < T < 1200)*

RED_P

$-1488.447 + 118.356409\ T - 23.3144\ T\ \ln(T) - 2.71613E\text{-}3\ T^2 + 11600\ T^{-1}$ *(298.15 < T < 1090)*
$-4672.913 + 159.602773\ T - 29.216037\ T\ \ln(T)$ *(1090 < T < 1200)*

Data relative to RHOMBOHEDRAL_A7

LIQUID

$24442.9 - 22.424679\ T$ *(298.15 < T < 1200)*

BCC_A2

$24874 - 16.1\ T$ *(298.15 < T < 1200)*

FCC_A1

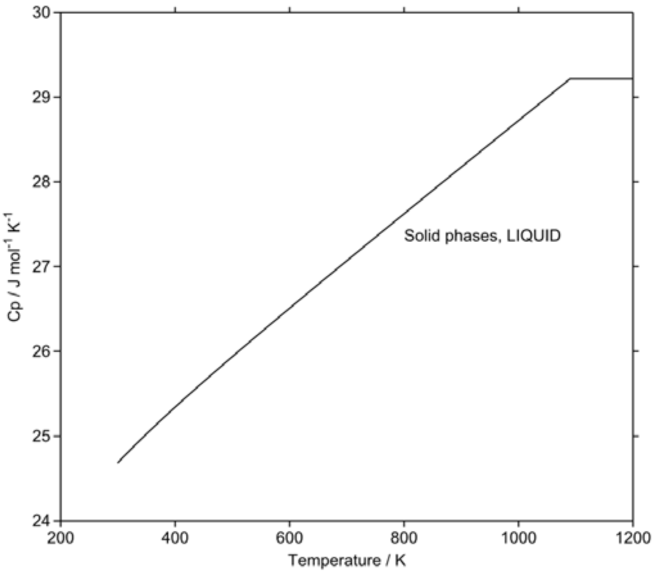
$24874 - 14.74\ T$ *(298.15 < T < 1200)*

HCP_A3

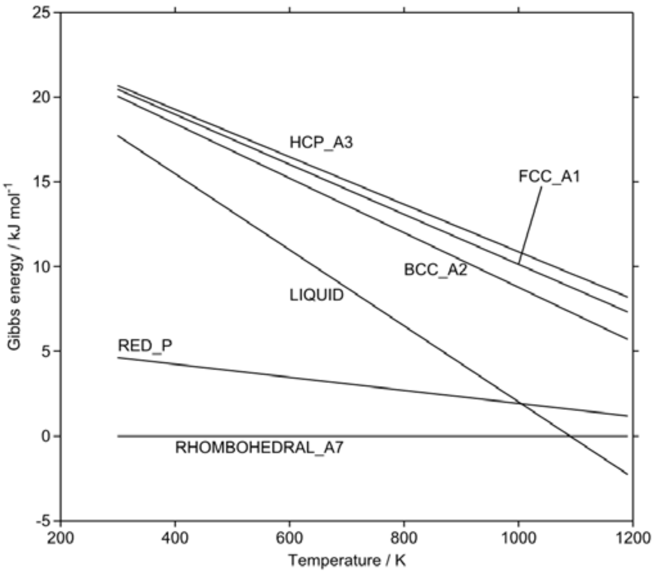
$24874 - 14\ T$ *(298.15 < T < 1200)*

RED_P

$5782 - 3.85466\ T$ *(298.15 < T < 1200)*



Heat capacity of As



Gibbs energy of phases of As relative to RHOMBOHEDRAL_A7

Au

Source of data: *Hultgren, revised by M H Rand [FCC_A1, LIQUID]*
I Ansara, M H Rand - unpublished work [HCP_A3]
Saunders et al. [BCC_A2]
J. Wang, X-G Lu, B. Sundman, X. Su, J. Alloys and Compounds, 2004, 364, 117-120 [DHCP]

FCC_A1

$-6938.856 + 106.830098\ T - 22.75455\ T\ln(T) - 3.85924E\text{-}3\ T^2 + 0.379625E\text{-}6\ T^3 - 25097\ T^{-1}$ *(298.15 < T < 929.4)*
$-93586.481 + 1021.69543\ T - 155.7067449\ T\ln(T) + 87.56015E\text{-}3\ T^2 - 11.518713E\text{-}6\ T^3 + 10637210\ T^{-1}$ *(929.4 < T < 1337.33)*
$314067.829 - 2016.378254\ T + 263.2522592\ T\ln(T) - 118.216828E\text{-}3\ T^2 + 8.923844E\text{-}6\ T^3 - 67999832\ T^{-1}$ *(1337.33 < T < 1735.8)*
$-12133.783 + 165.272524\ T - 30.9616\ T\ln(T)$ *(1735.8 < T < 3200)*

LIQUID

$5613.144 + 97.444232\ T - 22.75455\ T\ln(T) - 3.85924E\text{-}3\ T^2 + 0.379625E\text{-}6\ T^3 - 25097\ T^{-1}$ *(298.15 < T < 929.4)*
$-81034.481 + 1012.309564\ T - 155.7067449\ T\ln(T) + 87.56015E\text{-}3\ T^2 - 11.518713E\text{-}6\ T^3 + 10637210\ T^{-1}$ *(929.4 < T < 1337.33)*
$326619.829 - 2025.76412\ T + 263.2522592\ T\ln(T) - 118.216828E\text{-}3\ T^2 + 8.923844E\text{-}6\ T^3 - 67999832\ T^{-1}$ *(1337.33 < T < 1735.8)*
$418.217 + 155.886658\ T - 30.9616\ T\ln(T)$ *(1735.8 < T < 3200)*

BCC_A2

$-2688.856 + 105.730098\ T - 22.75455\ T\ln(T) - 3.85924E\text{-}3\ T^2 + 0.379625E\text{-}6\ T^3 - 25097\ T^{-1}$ *(298.15 < T < 929.4)*
$-89336.481 + 1020.59543\ T - 155.7067449\ T\ln(T) + 87.56015E\text{-}3\ T^2 - 11.518713E\text{-}6\ T^3 + 10637210\ T^{-1}$ *(929.4 < T < 1337.33)*
$318317.829 - 2017.478254\ T + 263.2522592\ T\ln(T) - 118.216828E\text{-}3\ T^2 + 8.923844E\text{-}6\ T^3 - 67999832\ T^{-1}$ *(1337.33 < T < 1735.8)*
$-7883.783 + 164.172524\ T - 30.9616\ T\ln(T)$ *(1735.8 < T < 3200)*

HCP_A3

$-6698.106 + 108.430098\ T - 22.75455\ T\ln(T) - 3.85924E\text{-}3\ T^2 + 0.379625E\text{-}6\ T^3 - 25097\ T^{-1}$ *(298.15 < T < 929.4)*
$-93345.731 + 1023.29543\ T - 155.7067449\ T\ln(T) + 87.56015E\text{-}3\ T^2 - 11.518713E\text{-}6\ T^3 + 10637210\ T^{-1}$ *(929.4 < T < 1337.33)*
$314308.579 - 2014.778254\ T + 263.2522592\ T\ln(T) - 118.216828E\text{-}3\ T^2 + 8.923844E\text{-}6\ T^3 - 67999832\ T^{-1}$ *(1337.33 < T < 1735.8)*
$-11893.033 + 166.872524\ T - 30.9616\ T\ln(T)$ *(1735.8 < T < 3200)*

DHCP

-1938.856 + 106.830098 T - 22.75455 T ln(T) - 3.85924E-3 T^2 + 0.379625E-6 T^3 - 25097 T^{-1}
(298.15 < T < 929.4)
-88586.481 + 1021.69543 T - 155.7067449 T ln(T) + 87.56015E-3 T^2 - 11.518713E-6 T^3
+ 10637210 T^{-1} *(929.4 < T < 1337.33)*
319067.829 - 2016.378254 T + 263.2522592 T ln(T) - 118.216828E-3 T^2 + 8.923844E-6 T^3
- 67999832 T^{-1} *(1337.33 < T < 1735.8)*
-7133.783 + 165.272524 T - 30.9616 T ln(T) *(1735.8 < T < 3200)*

Data relative to FCC_A1

LIQUID

12552 - 9.385866 T *(298.15 < T < 3200)*

BCC_A2

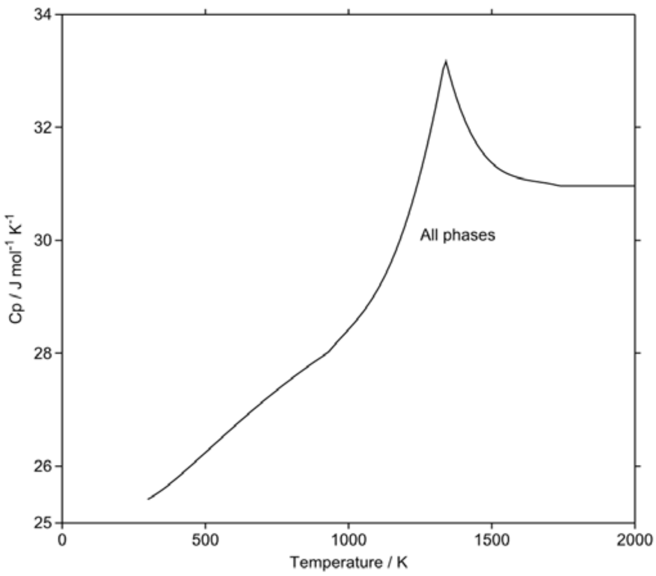
4250 - 1.1 T *(298.15 < T < 3200)*

HCP_A3

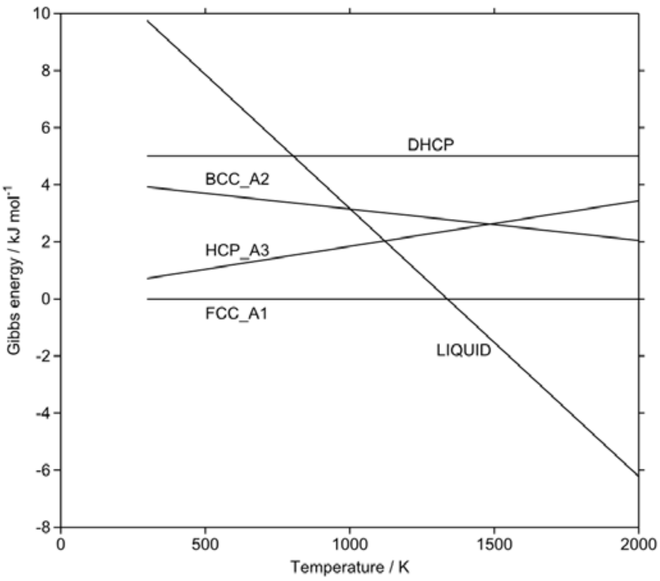
240.75 + 1.6 T *(298.15 < T < 3200)*

DHCP

5000 *(298.15 < T < 3200)*



Heat capacity of Au



Gibbs energy of phases of Au relative to FCC_A1

B

Source of data: *TPIS*

BETA_RHOMBO_B

$-7735.284 + 107.111864\ T - 15.6641\ T\ln(T) - 6.864515E\text{-}3\ T^2 + 0.618878E\text{-}6\ T^3 + 370843\ T^{-1}$ *(298.15 < T < 1100)*

$-16649.474 + 184.801744\ T - 26.6047\ T\ln(T) - 0.79809E\text{-}3\ T^2 - 0.02556E\text{-}6\ T^3 + 1748270\ T^{-1}$ *(1100 < T < 2348)*

$-36667.582 + 231.336244\ T - 31.5957527\ T\ln(T) - 1.59488E\text{-}3\ T^2 + 0.134719E\text{-}6\ T^3 + 11205883\ T^{-1}$ *(2348 < T < 3000)*

$-21530.653 + 222.396264\ T - 31.4\ T\ln(T)$ *(3000 < T < 6000)*

LIQUID

$40723.275 + 86.843839\ T - 15.6641\ T\ln(T) - 6.864515E\text{-}3\ T^2 + 0.618878E\text{-}6\ T^3 + 370843\ T^{-1}$ *(298.15 < T < 500)*

$41119.703 + 82.101722\ T - 14.9827763\ T\ln(T) - 7.095669E\text{-}3\ T^2 + 0.507347E\text{-}6\ T^3 + 335484\ T^{-1}$ *(500 < T < 2348)*

$28842.012 + 200.94731\ T - 31.4\ T\ln(T)$ *(2348 < T < 6000)*

DIAMOND_A4

$-7725.284 + 107.111864\ T - 15.6641\ T\ln(T) - 6.864515E\text{-}3\ T^2 + 0.618878E\text{-}6\ T^3 + 370843\ T^{-1}$ *(298.15 < T < 1100)*

$-16639.474 + 184.801744\ T - 26.6047\ T\ln(T) - 0.79809E\text{-}3\ T^2 - 0.02556E\text{-}6\ T^3 + 1748270\ T^{-1}$ *(1100 < T < 2348)*

$-36657.582 + 231.336244\ T - 31.5957527\ T\ln(T) - 1.59488E\text{-}3\ T^2 + 0.134719E\text{-}6\ T^3 + 11205883\ T^{-1}$ *(2348 < T < 3000)*

$-21520.653 + 222.396264\ T - 31.4\ T\ln(T)$ *(3000 < T < 6000)*

GRAPHITE

$2264.716 + 105.111864\ T - 15.6641\ T\ln(T) - 6.864515E\text{-}3\ T^2 + 0.618878E\text{-}6\ T^3 + 370843\ T^{-1}$ *(298.15 < T < 1100)*

$-6649.474 + 182.801744\ T - 26.6047\ T\ln(T) - 0.79809E\text{-}3\ T^2 - 0.02556E\text{-}6\ T^3 + 1748270\ T^{-1}$ *(1100 < T < 2348)*

$-26667.582 + 229.336244\ T - 31.5957527\ T\ln(T) - 1.59488E\text{-}3\ T^2 + 0.134719E\text{-}6\ T^3 + 11205883\ T^{-1}$ *(2348 < T < 3000)*

$-11530.653 + 220.396264\ T - 31.4\ T\ln(T)$ *(3000 < T < 6000)*

BCC_A2

$35778.716 + 94.894864\ T - 15.6641\ T\ln(T) - 6.864515E\text{-}3\ T^2 + 0.618878E\text{-}6\ T^3 + 370843\ T^{-1}$ *(298.15 < T < 1100)*

$26864.526 + 172.584744\ T - 26.6047\ T\ln(T) - 0.79809E\text{-}3\ T^2 - 0.02556E\text{-}6\ T^3 + 1748270\ T^{-1}$
(1100 < T < 2348)
$6846.418 + 219.119244\ T - 31.5957527\ T\ln(T) - 1.59488E\text{-}3\ T^2 + 0.134719E\text{-}6\ T^3 + 11205883\ T^{-1}$
(2348 < T < 3000)

FCC_A1

$35778.716 + 94.894864\ T - 15.6641\ T\ln(T) - 6.864515E\text{-}3\ T^2 + 0.618878E\text{-}6\ T^3 + 370843\ T^{-1}$
(298.15 < T < 1100)
$26864.526 + 172.584744\ T - 26.6047\ T\ln(T) - 0.79809E\text{-}3\ T^2 - 0.02556E\text{-}6\ T^3 + 1748270\ T^{-1}$
(1100 < T < 2348)
$6846.418 + 219.119244\ T - 31.5957527\ T\ln(T) - 1.59488E\text{-}3\ T^2 + 0.134719E\text{-}6\ T^3 + 11205883\ T^{-1}$
(2348 < T < 3000)
$21983.347 + 210.179264\ T - 31.4\ T\ln(T)$ *(3000 < T < 6000)*

HCP_A3

$42472.716 + 97.405864\ T - 15.6641\ T\ln(T) - 6.864515E\text{-}3\ T^2 + 0.618878E\text{-}6\ T^3 + 370843\ T^{-1}$
(298.15 < T < 1100)
$33558.526 + 175.095744\ T - 26.6047\ T\ln(T) - 0.79809E\text{-}3\ T^2 - 0.02556E\text{-}6\ T^3 + 1748270\ T^{-1}$
(1100 < T < 2348)
$13540.418 + 221.630244\ T - 31.5957527\ T\ln(T) - 1.59488E\text{-}3\ T^2 + 0.134719E\text{-}6\ T^3 + 11205883\ T^{-1}$
(2348 < T < 3000)
$28677.347 + 212.690264\ T - 31.4\ T\ln(T)$ *(3000 < T < 6000)*

Data relative to BETA_RHOMBO_B

LIQUID

$48458.559 - 20.268025\ T$ *(298.15 < T < 500)*
$48854.987 - 25.010142\ T + 0.6813237\ T\ln(T) - 0.231154E\text{-}3\ T^2 - 0.111531E\text{-}6\ T^3 - 35359\ T^{-1}$
(500 < T < 1100)
$57769.177 - 102.700022\ T + 11.6219237\ T\ln(T) - 6.297579E\text{-}3\ T^2 + 0.532907E\text{-}6\ T^3 - 1412786\ T^{-1}$
(1100 < T < 2348)
$65509.594 - 30.388934\ T + 0.1957527\ T\ln(T) + 1.59488E\text{-}3\ T^2 - 0.134719E\text{-}6\ T^3 - 11205883\ T^{-1}$
(2348 < T < 3000)
$50372.665 - 21.448954\ T$ *(3000 < T < 6000)*

DIAMOND_A4

10 *(298.15 < T < 6000)*

GRAPHITE

$10000 - 2\ T$ *(298.15 < T < 6000)*

BCC_A2

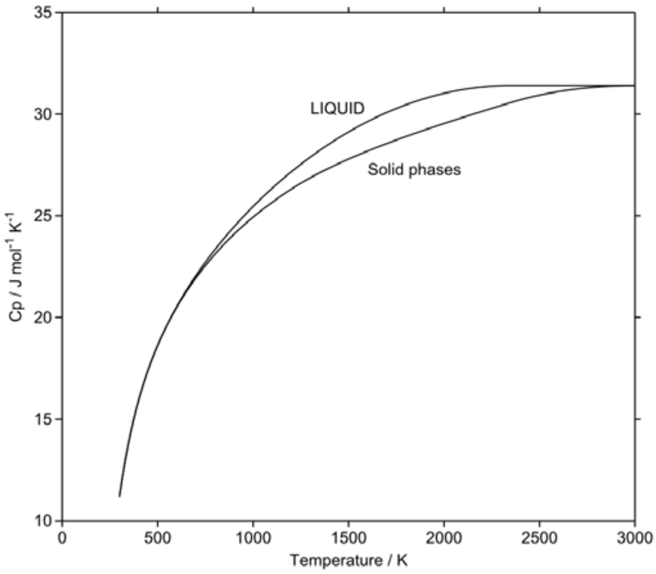
43514 - 12.217 T *(298.15 < T < 3000)*

FCC_A1

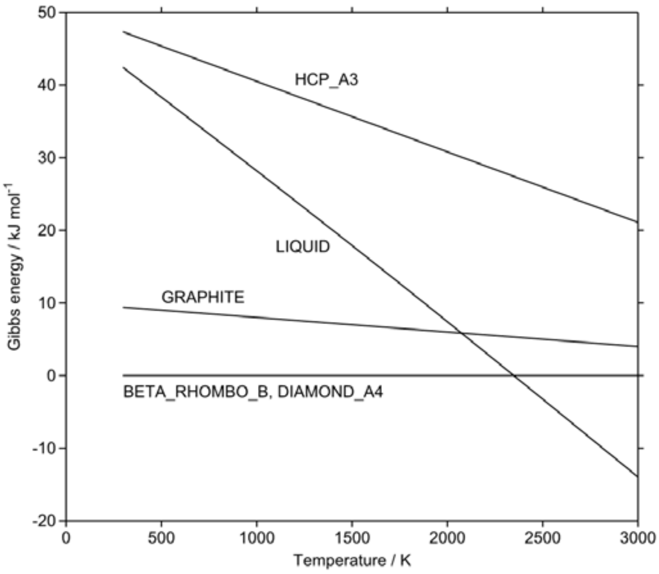
43514 - 12.217 T *(298.15 < T < 6000)*

HCP_A3

50208 - 9.706 T *(298.15 < T < 6000)*



Heat capacity of B



Gibbs energy of phases of B relative to BETA_RHOMBO_B

Ba

Source of data: *TPIS [BCC_A2, LIQUID]*
Saunders et al. [HCP_A3, FCC_A1]

BCC_A2

$-17685.226 + 233.78606\ T - 42.889\ T \ln(T) - 1.8314E\text{-}3\ T^2 - 0.000095E\text{-}6\ T^3 + 705880\ T^{-1}$
(298.15 < T < 1000)

$-64873.614 + 608.188389\ T - 94.2824199\ T \ln(T) + 19.504772E\text{-}3\ T^2 - 1.051353E\text{-}6\ T^3 + 8220192\ T^{-1}$
(1000 < T < 2995)

$8083.889 + 136.780042\ T - 32.2\ T \ln(T)$ *(2995 < T < 4000)*

LIQUID

$-9738.988 + 229.540143\ T - 43.4961089\ T\ \ln(T) - 2.346416E{-3}\ T^2 + 0.991223E{-6}\ T^3 + 723016\ T^{-1}$

(298.15 < T < 1000)

$-7381.093 + 235.49642\ T - 45.103\ T\ \ln(T) + 2.154E{-3}\ T^2 + 0.000027E{-6}\ T^3 - 365\ T^{-1}$

(1000 < T < 2995)

$11940.282 + 132.212\ T - 32.2\ T\ \ln(T)$ *(2995 < T < 4000)*

FCC_A1

$-15885.226 + 234.38606\ T - 42.889\ T\ \ln(T) - 1.8314E{-3}\ T^2 - 0.000095E{-6}\ T^3 + 705880\ T^{-1}$

(298.15 < T < 1000)

$-63073.614 + 608.788389\ T - 94.2824199\ T\ \ln(T) + 19.504772E{-3}\ T^2 - 1.051353E{-6}\ T^3 + 8220192\ T^{-1}$

(1000 < T < 2995)

$9883.889 + 137.380042\ T - 32.2\ T\ \ln(T)$ *(2995 < T < 4000)*

HCP_A3

$-15685.226 + 235.08606\ T - 42.889\ T\ \ln(T) - 1.8314E{-3}\ T^2 - 0.000095E{-6}\ T^3 + 705880\ T^{-1}$

(298.15 < T < 1000)

$-62873.614 + 609.488389\ T - 94.2824199\ T\ \ln(T) + 19.504772E{-3}\ T^2 - 1.051353E{-6}\ T^3 + 8220192\ T^{-1}$

(1000 < T < 2995)

$10083.889 + 138.080042\ T - 32.2\ T\ \ln(T)$ *(2995 < T < 4000)*

Data relative to BCC_A2

LIQUID

$7946.238 - 4.245917\ T - 0.6071089\ T\ \ln(T) - 0.515016E{-3}\ T^2 + 0.991318E{-6}\ T^3 + 17136\ T^{-1}$

(298.15 < T < 1000)

$57492.521 - 372.691969\ T + 49.1794199\ T\ \ln(T) - 17.350772E{-3}\ T^2 + 1.05138E{-6}\ T^3 - 8220557\ T^{-1}$

(1000 < T < 2995)

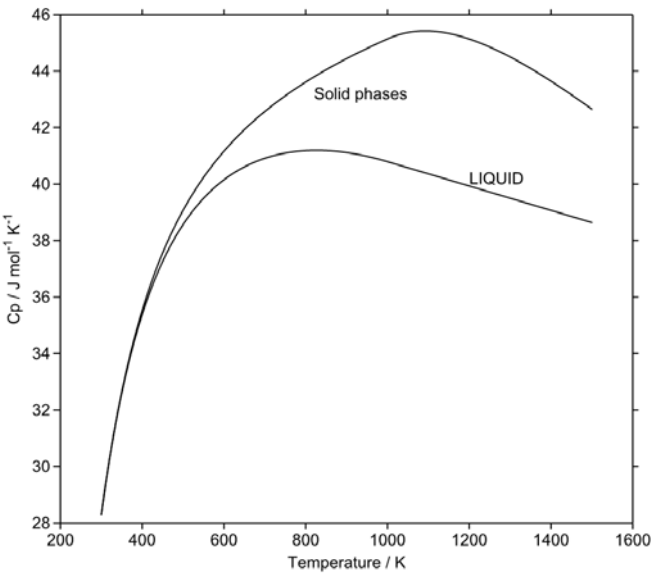
$3856.393 - 4.568042\ T$ *(2995 < T < 4000)*

FCC_A1

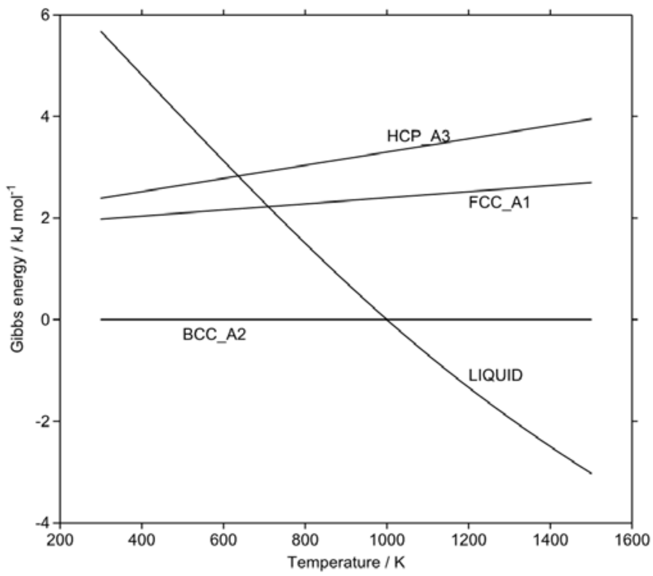
$1800 + 0.6\ T$ *(298.15 < T < 4000)*

HCP_A3

$2000 + 1.3\ T$ *(298.15 < T < 4000)*



Heat capacity of Ba



Gibbs energy of phases of Ba relative to BCC_A2

Be

Source of data: *JANAF, extended by A T Dinsdale [HCP_A3, BCC_A2, LIQUID]*
Saunders et al. [FCC_A1]

HCP_A3

$-8553.651 + 137.560219\ T - 21.204\ T\ \ln(T) - 2.84715E\text{-}3\ T^2 - 0.160413E\text{-}6\ T^3 + 293690\ T^{-1}$

(298.15 < T < 1527)

$-121305.858 + 772.405844\ T - 103.9842999\ T\ \ln(T) + 21.078651E\text{-}3\ T^2 - 1.119065E\text{-}6\ T^3 + 27251743\ T^{-1}$

(1527 < T < 3000)

BCC_A2

$-1076.057 + 109.411712\ T - 17.1727841\ T\ \ln(T) - 8.672487E\text{-}3\ T^2 + 0.961427E\text{-}6\ T^3 + 242309\ T^{-1}$

(298.15 < T < 1527)

$-6970.378 + 196.411689\ T - 30\ T\ \ln(T)$ *(1527 < T < 1560)*

$-2609.973 + 178.131722\ T - 27.7823769\ T\ \ln(T) - 0.103629E\text{-}3\ T^2 - 0.059331E\text{-}6\ T^3 - 1250847\ T^{-1}$

(1560 < T < 3000)

LIQUID

$7511.838 + 120.362788\ T - 20.0497038\ T\ \ln(T) - 4.821347E\text{-}3\ T^2 + 0.415958E\text{-}6\ T^3 + 281044\ T^{-1}$

(298.15 < T < 1560)

$5364.713 + 156.961141\ T - 25.486\ T\ \ln(T) - 1.0572E\text{-}3\ T^2 - 0.001117E\text{-}6\ T^3 + 15920\ T^{-1}$

(1560 < T < 3000)

FCC_A1

$-2204.651 + 136.475219\ T - 21.204\ T \ln(T) - 2.84715E\text{-}3\ T^2 - 0.160413E\text{-}6\ T^3 + 293690\ T^{-1}$ *(298.15 < T < 1527)*

$-114956.858 + 771.320844\ T - 103.9842999\ T \ln(T) + 21.078651E\text{-}3\ T^2 - 1.119065E\text{-}6\ T^3 + 27251743\ T^{-1}$ *(1527 < T < 3000)*

Data relative to HCP_A3

BCC_A2

$7477.594 - 28.148507\ T + 4.0312159\ T \ln(T) - 5.825337E\text{-}3\ T^2 + 1.12184E\text{-}6\ T^3 - 51381\ T^{-1}$ *(298.15 < T < 1527)*

$114335.48 - 575.994155\ T + 73.9842999\ T \ln(T) - 21.078651E\text{-}3\ T^2 + 1.119065E\text{-}6\ T^3 - 27251743\ T^{-1}$ *(1527 < T < 1560)*

$118695.885 - 594.274122\ T + 76.201923\ T \ln(T) - 21.18228E\text{-}3\ T^2 + 1.059734E\text{-}6\ T^3 - 28502590\ T^{-1}$ *(1560 < T < 3000)*

LIQUID

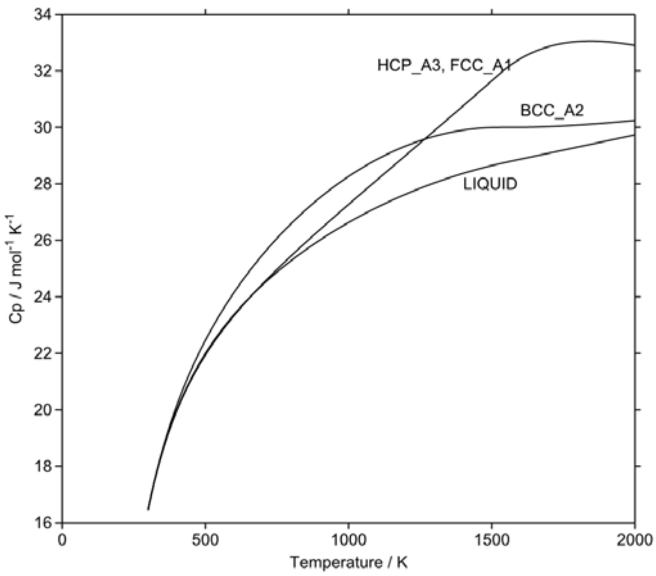
$16065.489 - 17.197431\ T + 1.1542962\ T \ln(T) - 1.974197E\text{-}3\ T^2 + 0.576371E\text{-}6\ T^3 - 12646\ T^{-1}$ *(298.15 < T < 1527)*

$128817.696 - 652.043056\ T + 83.9345961\ T \ln(T) - 25.899998E\text{-}3\ T^2 + 1.535023E\text{-}6\ T^3 - 26970699\ T^{-1}$ *(1527 < T < 1560)*

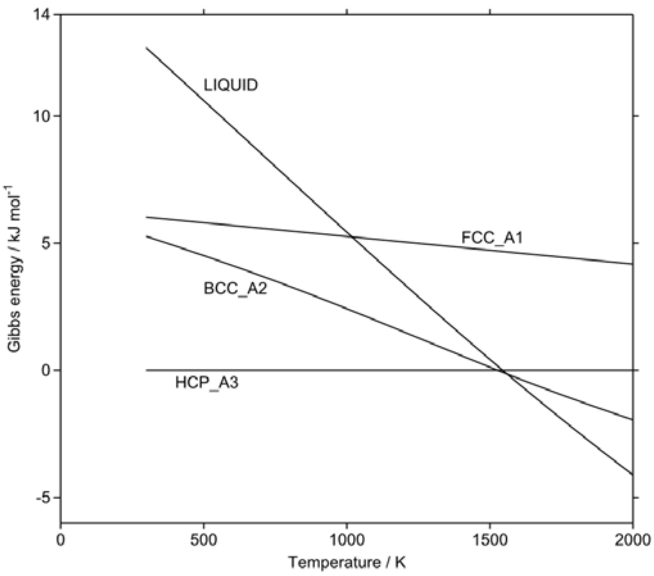
$126670.571 - 615.444703\ T + 78.4982999\ T \ln(T) - 22.135851E\text{-}3\ T^2 + 1.117948E\text{-}6\ T^3 - 27235823\ T^{-1}$ *(1560 < T < 3000)*

FCC_A1

$6349 - 1.085\ T$ *(298.15 < T < 3000)*



Heat capacity of Be



Gibbs energy of phases of Be relative to HCP_A3

Bi

Source of data: *Hultgren [RHOMBO_A7, LIQUID]*
P Y Chevalier [TETRAGONAL_A6, BCT_A5, TET_ALPHA1, DIAMOND_A4]
Saunders et al. [BCC_A2, FCC_A1, HCP_A3]

RHOMBOHEDRAL_A7

$-7817.776 + 128.418925\ T - 28.4096529\ T \ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*

$30208.022 - 393.650351\ T + 51.8556592\ T \ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 166.145E23\ T^{-9}$ *(544.55 < T < 800)*

$-11045.664 + 182.548971\ T - 35.9824\ T \ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3 + 166.145E23\ T^{-9}$ *(800 < T < 1200)*

$-7581.312 + 124.77144\ T - 27.196\ T \ln(T) + 166.145E23\ T^{-9}$ *(1200 < T < 3000)*

LIQUID

$3428.29 + 107.782416\ T - 28.4096529\ T \ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3 - 59.549E\text{-}20\ T^7$ *(298.15 < T < 544.55)*

$41544.282 - 414.460769\ T + 51.8556592\ T \ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1}$ *(544.55 < T < 800)*

$290.595 + 161.738553\ T - 35.9824\ T \ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3$ *(800 < T < 1200)*

$3754.947 + 103.961021\ T - 27.196\ T \ln(T)$ *(1200 < T < 3000)*

BCT_A5

$-3633.706 + 128.418925\ T - 28.4096529\ T \ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*

$34392.092 - 393.650351\ T + 51.8556592\ T \ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 166.145E23\ T^{-9}$ *(544.55 < T < 800)*

$-6861.594 + 182.548971\ T - 35.9824\ T \ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3 + 166.145E23\ T^{-9}$ *(800 < T < 1200)*

$-3397.242 + 124.77144\ T - 27.196\ T \ln(T) + 166.145E23\ T^{-9}$ *(1200 < T < 3000)*

TETRAGONAL_A6

$-3633.706 + 128.418925\ T - 28.4096529\ T \ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*

$34392.092 - 393.650351\ T + 51.8556592\ T \ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 166.145E23\ T^{-9}$ *(544.55 < T < 800)*

$-6861.594 + 182.548971\ T - 35.9824\ T \ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3 + 166.145E23\ T^{-9}$ *(800 < T < 1200)*

$-3397.242 + 124.77144\ T - 27.196\ T \ln(T) + 166.145E23\ T^{-9}$ *(1200 < T < 3000)*

TET_ALPHA1

$-3583.776 + 128.418925\ T - 28.4096529\ T\ \ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*

$34442.022 - 393.650351\ T + 51.8556592\ T\ \ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 166.145E23\ T^{-9}$ *(544.55 < T < 800)*

$-6811.664 + 182.548971\ T - 35.9824\ T\ \ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3 + 166.145E23\ T^{-9}$ *(800 < T < 1200)*

$-3347.312 + 124.77144\ T - 27.196\ T\ \ln(T) + 166.145E23\ T^{-9}$ *(1200 < T < 3000)*

BCC_A2

$3479.224 + 114.518925\ T - 28.4096529\ T\ \ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*

$41505.022 - 407.550351\ T + 51.8556592\ T\ \ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 166.145E23\ T^{-9}$ *(544.55 < T < 800)*

$251.336 + 168.648971\ T - 35.9824\ T\ \ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3 + 166.145E23\ T^{-9}$ *(800 < T < 1200)*

$3715.688 + 110.87144\ T - 27.196\ T\ \ln(T) + 166.145E23\ T^{-9}$ *(1200 < T < 3000)*

FCC_A1

$2082.224 + 115.918925\ T - 28.4096529\ T\ \ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*

$40108.022 - 406.150351\ T + 51.8556592\ T\ \ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 166.145E23\ T^{-9}$ *(544.55 < T < 800)*

$-1145.664 + 170.048971\ T - 35.9824\ T\ \ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3 + 166.145E23\ T^{-9}$ *(800 < T < 1200)*

$2318.688 + 112.27144\ T - 27.196\ T\ \ln(T) + 166.145E23\ T^{-9}$ *(1200 < T < 3000)*

HCP_A3

$2082.224 + 116.618925\ T - 28.4096529\ T\ \ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*

$40108.022 - 405.450351\ T + 51.8556592\ T\ \ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 166.145E23\ T^{-9}$ *(544.55 < T < 800)*

$-1145.664 + 170.748971\ T - 35.9824\ T\ \ln(T) + 7.4266E\text{-}3\ T^2 - 1.046E\text{-}6\ T^3 + 166.145E23\ T^{-9}$ *(800 < T < 1200)*

$2318.688 + 112.97144\ T - 27.196\ T\ \ln(T) + 166.145E23\ T^{-9}$ *(1200 < T < 3000)*

DIAMOND_A4

$3479.024 + 137.672580\ T - 28.4096529\ T\ \ln(T) + 12.338888E\text{-}3\ T^2 - 8.381598E\text{-}6\ T^3$ *(298.15 < T < 544.55)*

$41504.822 - 384.396696\ T + 51.8556592\ T\ \ln(T) - 75.311163E\text{-}3\ T^2 + 13.499885E\text{-}6\ T^3 - 3616168\ T^{-1} + 166.145E23\ T^{-9}$ *(544.55 < T < 800)*

$251.136 + 191.802626\ T - 35.9824\ T\ \ln(T) + 7.4266E{-3}\ T^2 - 1.046E{-6}\ T^3 + 166.145E23\ T^{-9}$ *(800 < T < 1200)*

$3715.488 + 134.025095\ T - 27.196\ T\ \ln(T) + 166.145E23\ T^{-9}$ *(1200 < T < 3000)*

Data relative to RHOMBOHEDRAL_A7

LIQUID

$11246.066 - 20.636509\ T - 59.549E{-20}\ T^7$ *(298.15 < T < 544.55)*

$11336.259 - 20.810418\ T - 166.145E23\ T^{-9}$ *(544.55 < T < 3000)*

BCT_A5

4184.07 *(298.15 < T < 3000)*

TETRAGONAL_A6

4184.07 *(298.15 < T < 3000)*

TET_ALPHA1

4234 *(298.15 < T < 3000)*

BCC_A2

11297 - 13.9 T *(298.15 < T < 3000)*

FCC_A1

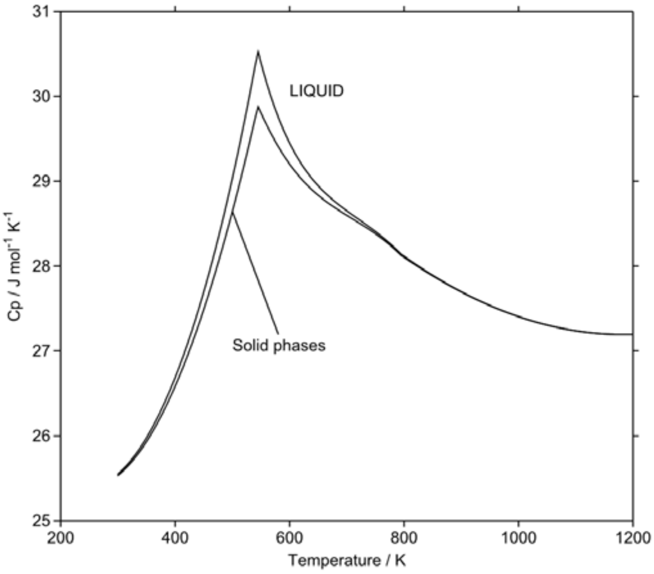
9900 - 12.5 T *(298.15 < T < 3000)*

HCP_A3

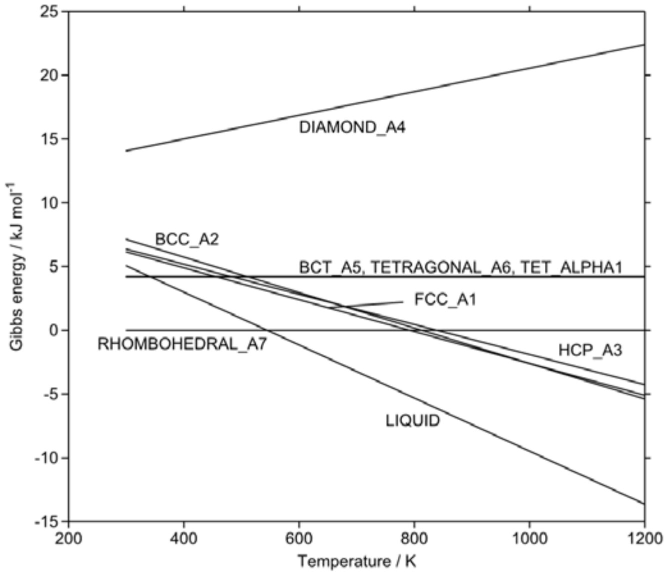
9900 - 11.8 T *(298.15 < T < 3000)*

DIAMOND_A4

11296.8 + 9.253655 T *(298.15 < T < 3000)*



Heat capacity of Bi



Gibbs energy of phases of Bi relative to RHOMBOHEDRAL_A7

C

Source of data: *P Gustafson, Carbon, 1986, **24**, 169-76*

GRAPHITE

$A = 5.259E-6$ $a_0 = 2.32E-5$ $a_1 = 5.7E-9$
$K_0 = 3.0E-11$ $n = 12$

$$-17368.441 + 170.73\,T - 24.3\,T\ln(T) - 0.4723E-3\,T^2 + 2562600\,T^{-1} - 2.643E8\,T^{-2} + 1.2E10\,T^{-3} + Gpres$$

(298.15 < T < 6000)

LIQUID

$A = 7.626E-6$ $a_0 = 2.32E-5$ $a_1 = 5.7E-9$
$K_0 = 1.6E-10$ $n = 2$

$$100000.559 + 146.1\,T - 24.3\,T\ln(T) - 0.4723E-3\,T^2 + 2562600\,T^{-1} - 2.643E8\,T^{-2} + 1.2E10\,T^{-3} + Gpres$$

(298.15 < T < 6000)

DIAMOND_A4

$A = 3.412E-6$ $a_0 = 2.43E-6$ $a_1 = 1.0E-8$
$K_0 = 1.7E-12$ $n = 5$

$$-16359.441 + 175.61\,T - 24.31\,T\ln(T) - 0.4723E-3\,T^2 + 2698000\,T^{-1} - 2.61E8\,T^{-2} + 1.11E10\,T^{-3} + Gpres$$

(298.15 < T < 6000)

Data relative to GRAPHITE

GRAPHITE

A = 5.259E-6	a_0 = 2.32E-5	a_1 = 5.7E-9
K_0 = 3.0E-11	n = 12	

Gpres *(298.15 < T < 6000)*

DIAMOND_A4

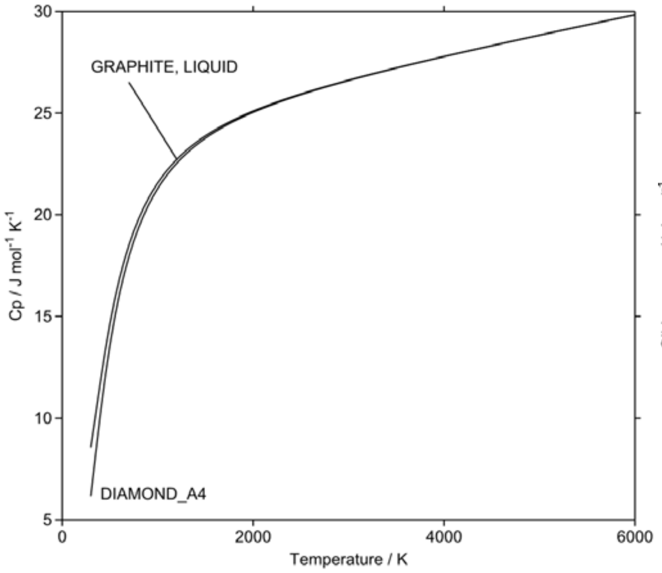
A = 3.412E-6	a_0 = 2.43E-6	a_1 = 1.0E-8
K_0 = 1.7E-12	n = 5	

$1009 + 4.88\ T - 0.01\ T\ln(T) + 135400\ T^{-1} + 33.0E5\ T^{-2} - 9E8\ T^{-3}$+Gpres *(298.15 < T < 6000)*

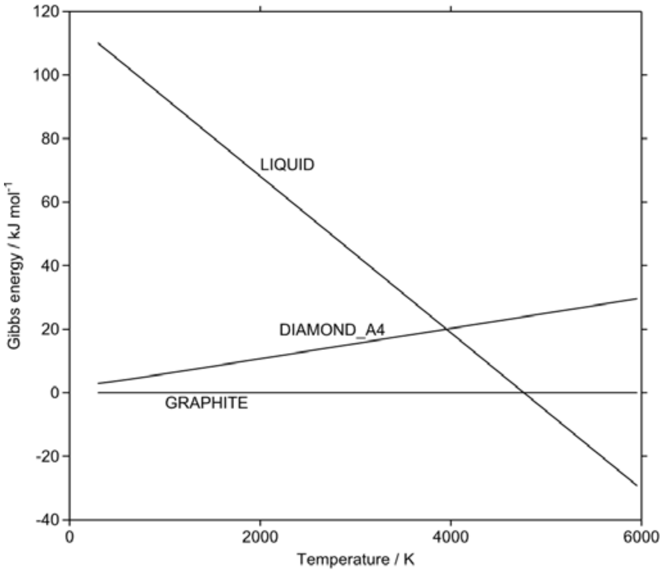
LIQUID

A = 7.626E-6	a_0 = 2.32E-5	a_1 = 5.7E-9
K_0 = 1.6E-10	n = 2	

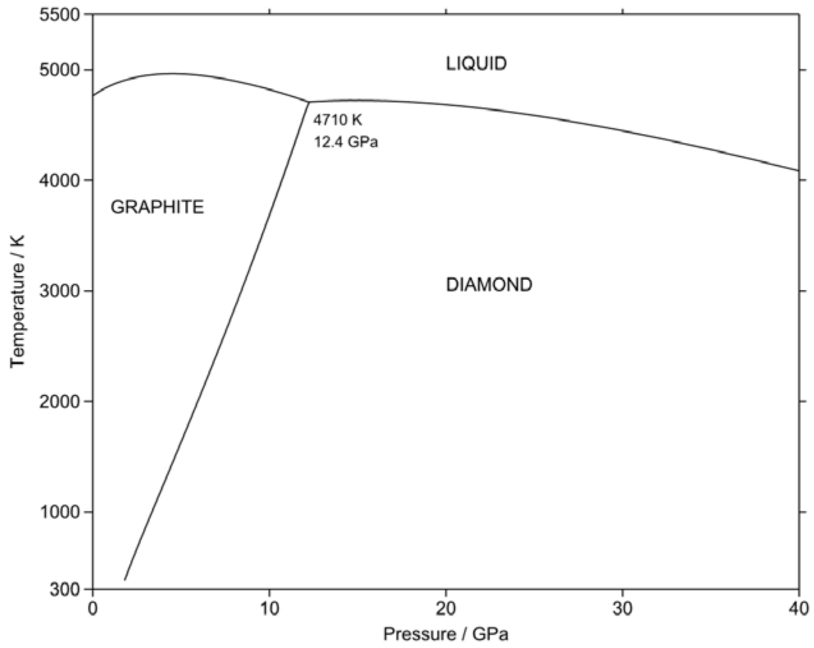
117369 - 24.63 T+Gpres *(298.15 < T < 6000)*



Heat capacity of C



Gibbs energy of phases of C relative to GRAPHITE



P-T phase diagram for C

Ca

Source of data : *CODATA extended by A T Dinsdale [FCC_A1, BCC_A2, LIQUID]*
Saunders et al. [HCP_A3]

FCC_A1

-4955.062 + 72.794266 T - 16.3138 T ln(T) - 11.10455E-3 T^2 - 133574 T^{-1} *(298.15 < T < 1115)*
-107304.428 + 799.982066 T - 114.2922467 T ln(T) + 23.733814E-3 T^2 - 1.2438E-6 T^3 + 18245540 T^{-1}
(1115 < T < 3000)
-3703.12 + 192.63995 T - 35 T ln(T) *(3000 < T < 3001)*

BCC_A2

-7020.852 + 142.970155 T - 28.2541 T ln(T) + 7.2326E-3 T^2 - 4.500217E-6 T^3 + 60578 T^{-1}
(298.15 < T < 716)
1640.475 + 1.999694 T - 6.276 T ln(T) - 16.1921E-3 T^2 - 523000 T^{-1} *(716 < T < 1115)*
-142331.096 + 1023.549046 T - 143.8726979 T ln(T) + 32.543127E-3 T^2 - 1.704079E-6 T^3
+ 25353771 T^{-1} *(1115 < T < 3000)*
321.63 + 189.433057 T - 35 T ln(T) *(3000 < T < 3001)*

LIQUID

5844.846 + 62.4838 T - 16.3138 T ln(T) - 11.10455E-3 T^2 - 133574 T^{-1} *(298.15 < T < 500)*
7838.856 + 18.2979 T - 8.9874787 T ln(T) - 22.66537E-3 T^2 + 3.338303E-6 T^3 - 230193 T^{-1}
(500 < T < 1115)

$-2654.938 + 188.9223\ T - 35\ T \ln(T)$ *(1115 < T < 3001)*

HCP_A3

$-4455.062 + 73.494266\ T - 16.3138\ T \ln(T) - 11.10455E{-3}\ T^2 - 133574\ T^{-1}$ *(298.15 < T < 1115)*
$-106804.428 + 800.682066\ T - 114.2922467\ T \ln(T) + 23.733814E{-3}\ T^2 - 1.2438E{-6}\ T^3 + 18245540\ T^{-1}$
(1115 < T < 3000)
$-3203.12 + 193.33995\ T - 35\ T \ln(T)$ *(3000 < T < 3001)*

Data relative to FCC_A1

BCC_A2

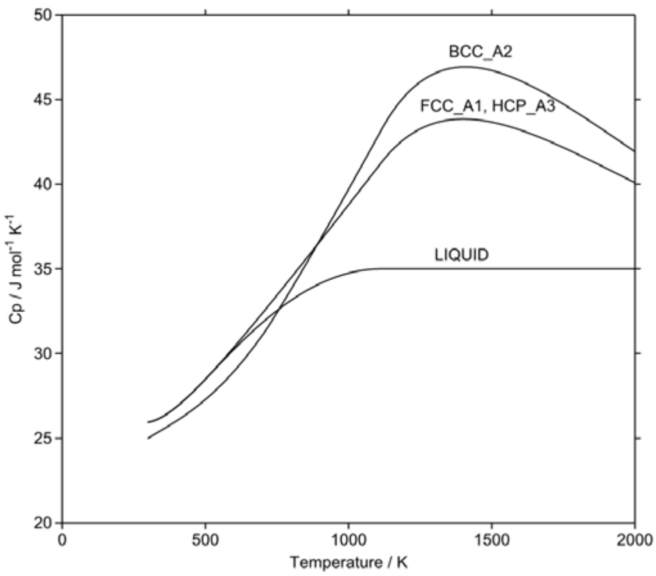
$-2065.79 + 70.175889\ T - 11.9403\ T \ln(T) + 18.33715E{-3}\ T^2 - 4.500217E{-6}\ T^3 + 194152\ T^{-1}$
(298.15 < T < 716)
$6595.537 - 70.794572\ T + 10.0378\ T \ln(T) - 5.08755E{-3}\ T^2 - 389426\ T^{-1}$ *(716 < T < 1115)*
$-35026.668 + 223.56698\ T - 29.5804512\ T \ln(T) + 8.809313E{-3}\ T^2 - 0.460279E{-6}\ T^3 + 7108231\ T^{-1}$
(1115 < T < 3000)
$4024.75 - 3.206893\ T$ *(3000 < T < 3001)*

LIQUID

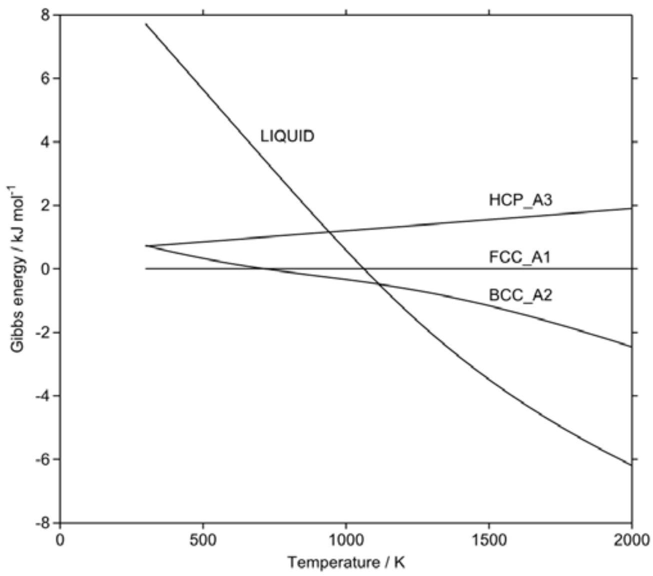
$10799.908 - 10.310466\ T$ *(298.15 < T < 500)*
$12793.918 - 54.496366\ T + 7.3263213\ T \ln(T) - 11.56082E{-3}\ T^2 + 3.338303E{-6}\ T^3 - 96619\ T^{-1}$
(500 < T < 1115)
$104649.49 - 611.059766\ T + 79.2922467\ T \ln(T) - 23.733814E{-3}\ T^2 + 1.2438E{-6}\ T^3 - 18245540\ T^{-1}$
(1115 < T < 3000)
$1048.182 - 3.71765\ T$ *(3000 < T < 3001)*

HCP_A3

$500 + 0.7\ T$ *(298.15 < T < 3001)*



Heat capacity of Ca



Gibbs energy of phases of Ca relative to FCC_A1

Cd

Source of data: *Hultgren [HCP_A3, LIQUID]*
J Jang,N J Silk, A Watson, A W Bryant, T G Chart, B B Argent, CALPHAD, 1995, 19(3), 415 [RHOMBO_A10, BCT_A5]
W Zakulski,Z Moser, K Rzyman,H L Lukas, S G Fries, M Sikiennik, R Kaczmarczyk, R Casternet;. J. Phase Equil. 1993,14(2),184-196 [FCC_A1, TETRAGONAL_A6]

BCT_A5

$-2083.469 + 99.506198\ T - 22.0442408\ T\ln(T) - 6.273908E{-3}\ T^2 - 6966\ T^{-1}$ *(298.15 < T < 594.22)*
$-15064.971 + 256.812233\ T - 45.1611543\ T\ln(T) + 8.832011E{-3}\ T^2 - 0.899604E{-6}\ T^3 + 1241290\ T^{-1}$ *(594.22 < T < 1500)*
$-4027.489 + 148.20548\ T - 29.7064\ T\ln(T)$ *(1500 < T < 1600)*

LIQUID

$-955.025 + 89.209282\ T - 22.0442408\ T\ln(T) - 6.273908E{-3}\ T^2 - 6966\ T^{-1}$ *(298.15 < T < 400)*
$21716.884 - 371.046869\ T + 53.1313898\ T\ln(T) - 115.159917E{-3}\ T^2 + 28.899781E{-6}\ T^3 - 1271815\ T^{-1}$ *(400 < T < 594.22)*
$-3252.303 + 138.251107\ T - 29.7064\ T\ln(T)$ *(594.22 < T < 1600)*

RHOMBO_A10

$-6283.469 + 98.886198\ T - 22.0442408\ T\ln(T) - 6.273908E{-3}\ T^2 - 6966\ T^{-1}$ *(298.15 < T < 594.22)*
$-19264.971 + 256.192233\ T - 45.1611543\ T\ln(T) + 8.832011E{-3}\ T^2 - 0.899604E{-6}\ T^3 + 1241290\ T^{-1}$ *(594.22 < T < 1500)*
$-8227.489 + 147.58548\ T - 29.7064\ T\ln(T)$ *(1500 < T < 1600)*

TETRAGONAL_A6

$-6191.169 + 98.586198\,T - 22.0442408\,T\ln(T) - 6.273908E{-3}\,T^2 - 6966\,T^{-1}$ *(298.15 < T < 594.22)*
$-19172.671 + 255.892233\,T - 45.1611543\,T\ln(T) + 8.832011E{-3}\,T^2 - 0.899604E{-6}\,T^3 + 1241290\,T^{-1}$ *(594.22 < T < 1500)*
$-8135.189 + 147.28548\,T - 29.7064\,T\ln(T)$ *(1500 < T < 1600)*

FCC_A1

$-6191.169 + 98.586198\,T - 22.0442408\,T\ln(T) - 6.273908E{-3}\,T^2 - 6966\,T^{-1}$ *(298.15 < T < 594.22)*
$-19172.671 + 255.892233\,T - 45.1611543\,T\ln(T) + 8.832011E{-3}\,T^2 - 0.899604E{-6}\,T^3 + 1241290\,T^{-1}$ *(594.22 < T < 1500)*
$-8135.189 + 147.28548\,T - 29.7064\,T\ln(T)$ *(1500 < T < 1600)*

HCP_A3

$-7083.469 + 99.506198\,T - 22.0442408\,T\ln(T) - 6.273908E{-3}\,T^2 - 6966\,T^{-1}$ *(298.15 < T < 594.22)*
$-20064.971 + 256.812233\,T - 45.1611543\,T\ln(T) + 8.832011E{-3}\,T^2 - 0.899604E{-6}\,T^3 + 1241290\,T^{-1}$ *(594.22 < T < 1500)*
$-9027.489 + 148.20548\,T - 29.7064\,T\ln(T)$ *(1500 < T < 1600)*

BCC_A2

$-6083.469 + 99.506198\,T - 22.0442408\,T\ln(T) - 6.273908E{-3}\,T^2 - 6966\,T^{-1}$ *(298.15 < T < 594.22)*
$-19064.971 + 256.812233\,T - 45.1611543\,T\ln(T) + 8.832011E{-3}\,T^2 - 0.899604E{-6}\,T^3 + 1241290\,T^{-1}$ *(594.22 < T < 1500)*
$-8027.489 + 148.20548\,T - 29.7064\,T\ln(T)$ *(1500 < T < 1600)*

Data relative to HCP_A3

BCT_A5

5000 *(298.15 < T < 1600)*

LIQUID

$6128.444 - 10.296916\,T$ *(298.15 < T < 400)*
$28800.353 - 470.553067\,T + 75.1756306\,T\ln(T) - 108.886009E{-3}\,T^2 + 28.899781E{-6}\,T^3 - 1264849\,T^{-1}$ *(400 < T < 594.22)*
$16812.668 - 118.561126\,T + 15.4547543\,T\ln(T) - 8.832011E{-3}\,T^2 + 0.899604E{-6}\,T^3 - 1241290\,T^{-1}$ *(594.22 < T < 1500)*
$5775.186 - 9.954373\,T$ *(1500 < T < 1600)*

RHOMBO_A10

$800 - 0.62\,T$ *(298.15 < T < 1600)*

TETRAGONAL_A6

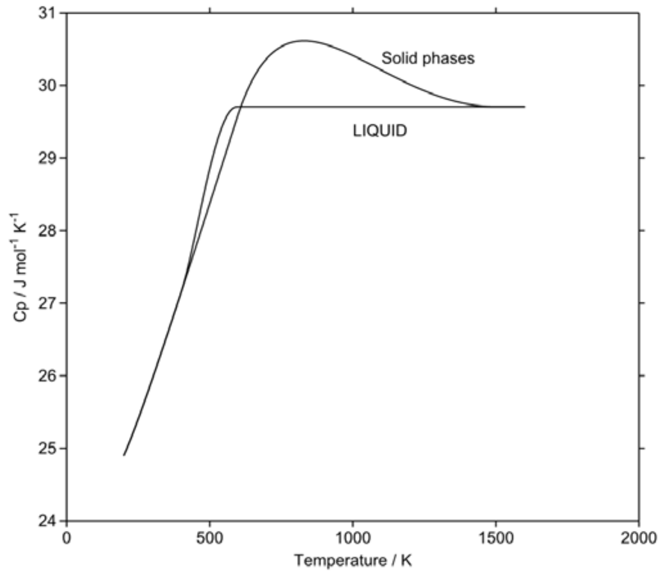
$892.3 - 0.92\,T$ *(298.15 < T < 1600)*

FCC_A1

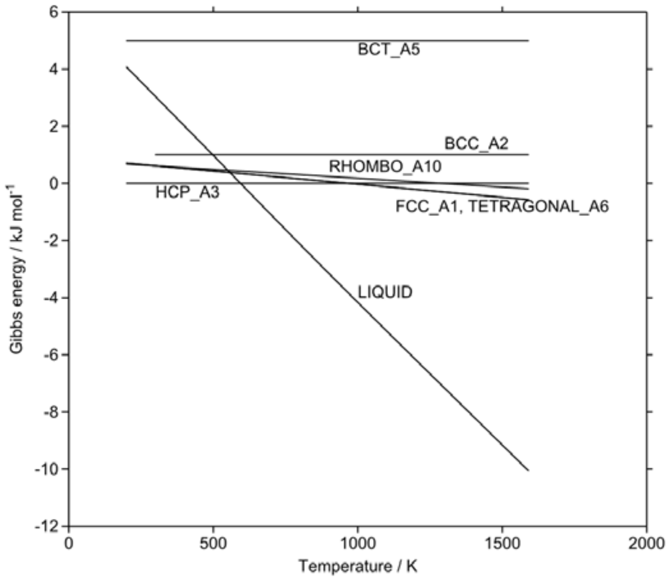
$892.3 - 0.92\,T$ *(298.15 < T < 1600)*

BCC_A2

1000 *(298.15 < T < 1600)*



Heat capacity of Cd



Gibbs energy of phases of Cd relative to HCP_A3

Ce

Source of data: *Hultgren extended by A T Dinsdale [FCC_A1, BCC_A2, LIQUID]*
P Franke (private communication) [HCP_A3]
K A Gschneider, V K Pecharsky; J Phase Equil.; 1999, 20(6), 612-4 [DHCP]

FCC_A1

$-7160.519 + 84.23022\,T - 22.3664\,T\ln(T) - 6.7103E\text{-}3\,T^2 - 0.320773E\text{-}6\,T^3 - 18117\,T^{-1}$
(298.15 < T < 1000)

$-79678.506 + 659.4604\,T - 101.3224803\,T\ln(T) + 26.046487E\text{-}3\,T^2 - 1.930297E\text{-}6\,T^3 + 11531707\,T^{-1}$
(1000 < T < 2000)

$-14198.639 + 190.370192\,T - 37.6978\,T\ln(T)$ *(2000 < T < 4000)*

DHCP

$-7283.058 + 84.66322\ T - 22.3664\ T \ln(T) - 6.7103E\text{-}3\ T^2 - 0.320773E\text{-}6\ T^3 - 18117\ T^{-1}$

(298.15 < T < 1000)

$-79801.045 + 659.8934\ T - 101.3224803\ T \ln(T) + 26.046487E\text{-}3\ T^2 - 1.930297E\text{-}6\ T^3 + 11531707\ T^{-1}$

(1000 < T < 2000)

$-14321.178 + 190.803192\ T - 37.6978\ T \ln(T)$ *(2000 < T < 4000)*

LIQUID

$4117.865 - 11.423898\ T - 7.5383948\ T \ln(T) - 29.36407E\text{-}3\ T^2 + 4.827734E\text{-}6\ T^3 - 198834\ T^{-1}$

(298.15 < T < 1000)

$-6730.605 + 183.023193\ T - 37.6978\ T \ln(T)$ *(1000 < T < 4000)*

BCC_A2

$-1354.69 - 5.21501\ T - 7.7305867\ T \ln(T) - 29.098402E\text{-}3\ T^2 + 4.784299E\text{-}6\ T^3 - 196303\ T^{-1}$

(298.15 < T < 1000)

$-12101.106 + 187.449688\ T - 37.6142\ T \ln(T)$ *(1000 < T < 1072)*

$-11950.375 + 186.333811\ T - 37.4627992\ T \ln(T) - 0.057145E\text{-}3\ T^2 + 0.002348E\text{-}6\ T^3 - 25897\ T^{-1}$

(1072 < T < 4000)

HCP_A3

$-6860.519 + 84.23022\ T - 22.3664\ T \ln(T) - 6.7103E\text{-}3\ T^2 - 0.320773E\text{-}6\ T^3 - 18117\ T^{-1}$

(298.15 < T < 1000)

$-79378.506 + 659.4604\ T - 101.3224803\ T \ln(T) + 26.046487E\text{-}3\ T^2 - 1.930297E\text{-}6\ T^3 + 11531707\ T^{-1}$

(1000 < T < 2000)

$-13898.639 + 190.370192\ T - 37.6978\ T \ln(T)$ *(2000 < T < 4000)*

Data relative to FCC_A1

DHCP

$-122.539 + 0.433\ T$ *(298.15 < T < 4000)*

LIQUID

$11278.384 - 95.654118\ T + 14.8280052\ T \ln(T) - 22.65377E\text{-}3\ T^2 + 5.148507E\text{-}6\ T^3 - 180717\ T^{-1}$

(298.15 < T < 1000)

$72947.901 - 476.437207\ T + 63.6246803\ T \ln(T) - 26.046487E\text{-}3\ T^2 + 1.930297E\text{-}6\ T^3 - 11531707\ T^{-1}$

(1000 < T < 2000)

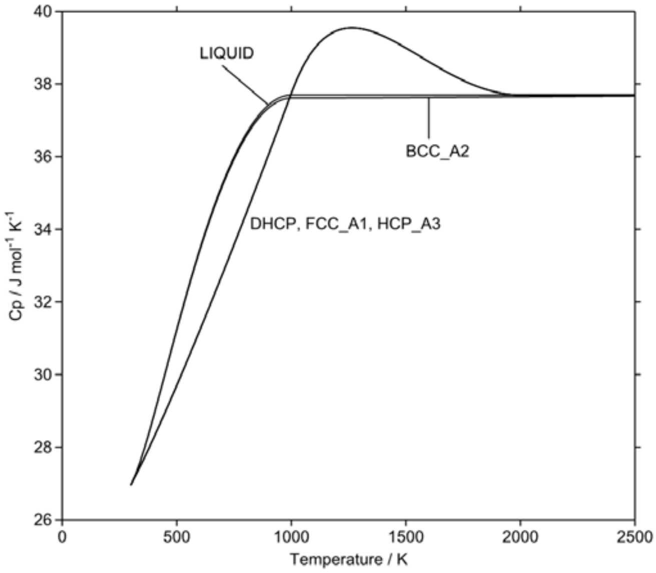
$7468.034 - 7.346999\ T$ *(2000 < T < 4000)*

BCC_A2

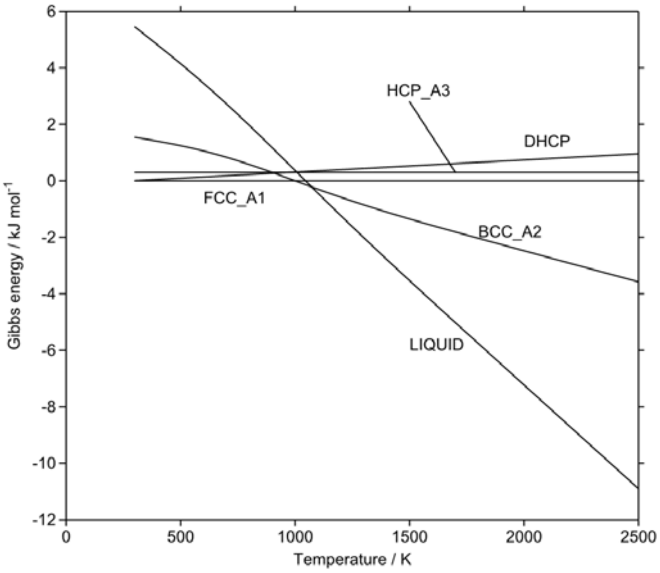
5805.829 - 89.44523 T + 14.6358133 T ln(T) - 22.388102E-3 T^2 + 5.105072E-6 T^3 - 178186 T^{-1}
(298.15 < T < 1000)
67577.4 - 472.010712 T + 63.7082803 T ln(T) - 26.046487E-3 T^2 + 1.930297E-6 T^3 - 11531707 T^{-1}
(1000 < T < 1072)
67728.131 - 473.126589 T + 63.8596811 T ln(T) - 26.103632E-3 T^2 + 1.932645E-6 T^3 - 11557604 T^{-1}
(1072 < T < 2000)
2248.264 - 4.036381 T + 0.2350008 T ln(T) - 0.057145E-3 T^2 + 0.002348E-6 T^3 - 25897 T^{-1}
(2000 < T < 4000)

HCP_A3

300 *(298.15 < T < 4000)*



Heat capacity of Ce



Gibbs energy of phases of Ce relative to FCC_A1

Co

Source of data: *A Fernandez Guillermet, Int. J. Thermophys., 1987, **8**(4), 481 [HCP_A3, FCC_A1, LIQUID]*
*A Fernandez Guillermet, High Temp. - High Press., 1987, **19**, 477-9 [BCC_A2]*
Weiming Huang, Report, TRITA-MAC-0386 [BCC_A12, CUB_A13]

HCP_A3

T_C = 1396 B_0 = 1.35
A = 6.719875E-6 a_0 = 3.4581936E-5 a_1 = 5.587534E-9
K_0 = 4.51216E-12 K_1 = 1.60731E-15 K_2 = 4.66729E-20 n = 4.007

310.241 + 133.36601 T - 25.0861 T ln(T) - 2.654739E-3 T^2 - 0.17348E-6 T^3 + 72527 T^{-1} +Gpres + Gmag *(298.15 < T < 1768)*

$-17197.666 + 253.28374\,T - 40.5\,T\ln(T) + 934.88E28\,T^{-9}$ +Gpres + Gmag *(1768 < T < 6000)*

LIQUID

A = 6.465079E-6 a_0 = 10.1216993E-5 a_1 = -8.3E-9
K_0 = 5.06842E-12 K_1 = 4.32538E-15 n = 4.5925

$15395.278 + 124.434078\,T - 25.0861\,T\ln(T) - 2.654739E\text{-}3\,T^2 - 0.17348E\text{-}6\,T^3 + 72527\,T^{-1}$
$- 219.801E\text{-}23\,T^7$ +Gpres *(298.15 < T < 1768)*
$-846.61 + 243.599944\,T - 40.5\,T\ln(T)$ +Gpres *(1768 < T < 6000)*

BCC_A2

T_C = 1450.0 B_0 = 1.35
A = 6.8147641E-6 a_0 = 3.20701588E-5 a_1 = 2.93417253E-9
K_0 = 4.66591978E-12 K_1 = 1.45932922E-15 K_2 = 5.173687E-20 n = 4.007

$3248.241 + 132.65221\,T - 25.0861\,T\ln(T) - 2.654739E\text{-}3\,T^2 - 0.17348E\text{-}6\,T^3 + 72527\,T^{-1}$ +Gpres
+ Gmag *(298.15 < T < 1768)*
$-14259.666 + 252.56994\,T - 40.5\,T\ln(T) + 934.88E28\,T^{-9}$ +Gpres + Gmag *(1768 < T < 6000)*

CBCC_A12

$4465.241 + 133.36601\,T - 25.0861\,T\ln(T) - 2.654739E\text{-}3\,T^2 - 0.17348E\text{-}6\,T^3 + 72527\,T^{-1}$
(298.15 < T < 1768)
$-13042.666 + 253.28374\,T - 40.5\,T\ln(T) + 934.88E28\,T^{-9}$ *(1768 < T < 6000)*

CUB_A13

$3465.241 + 133.36601\,T - 25.0861\,T\ln(T) - 2.654739E\text{-}3\,T^2 - 0.17348E\text{-}6\,T^3 + 72527\,T^{-1}$
(298.15 < T < 1768)
$-14042.666 + 253.28374\,T - 40.5\,T\ln(T) + 934.88E28\,T^{-9}$ *(1768 < T < 6000)*

FCC_A1

T_C = 1396 B_0 = 1.35
A = 6.752927E-6 a_0 = 3.2070159E-5 a_1 = 5.868345E-9
K_0 = 4.66592E-12 K_1 = 1.45933E-15 K_2 = 5.17369E-20 n = 4.007

$737.832 + 132.750762\,T - 25.0861\,T\ln(T) - 2.654739E\text{-}3\,T^2 - 0.17348E\text{-}6\,T^3 + 72527\,T^{-1}$ +Gpres
+ Gmag *(298.15 < T < 1768)*
$-16770.075 + 252.668492\,T - 40.5\,T\ln(T) + 934.88E28\,T^{-9}$ +Gpres + Gmag *(1768 < T < 6000)*

Data relative to paramagnetic HCP_A3

HCP_A3

$T_C = 1396$ $\quad B_0 = 1.35$
$A = 6.719875E\text{-}6$ $\quad a_0 = 3.4581936E\text{-}5$ $\quad a_1 = 5.587534E\text{-}9$
$K_0 = 4.51216E\text{-}12$ $\quad K_1 = 1.60731E\text{-}15$ $\quad K_2 = 4.66729E\text{-}20$ $\quad n = 4.007$

Gpres + Gmag *(298.15 < T < 6000)*

LIQUID

$A = 6.465079E\text{-}6$ $\quad a_0 = 10.1216993E\text{-}5$ $\quad a_1 = -8.3E\text{-}9$
$K_0 = 5.06842E\text{-}12$ $\quad K_1 = 4.32538E\text{-}15$ $\quad n = 4.5925$

$15085.037 - 8.931932\ T - 219.801E\text{-}23\ T^7$ +Gpres *(298.15 < T < 1768)*
$16351.056 - 9.683796\ T - 934.88E28\ T^{-9}$ +Gpres *(1768 < T < 6000)*

BCC_A2

$T_C = 1450.0$ $\quad B_0 = 1.35$
$A = 6.8147641E\text{-}6$ $\quad a_0 = 3.2070159E\text{-}5$ $\quad a_1 = 2.93417253E\text{-}9$
$K_0 = 4.66592E\text{-}12$ $\quad K_1 = 1.45933E\text{-}15$ $\quad K_2 = 5.17369E\text{-}20$ $\quad n = 4.007$

2938 - 0.7138 T +Gpres + Gmag *(298.15 < T < 6000)*

CBCC_A12

4155 *(298.15 < T < 6000)*

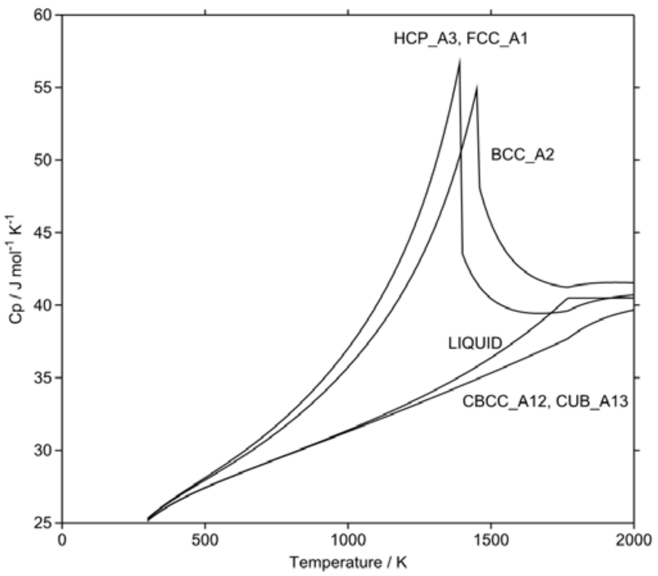
CUB_A13

3155 *(298.15 < T < 6000)*

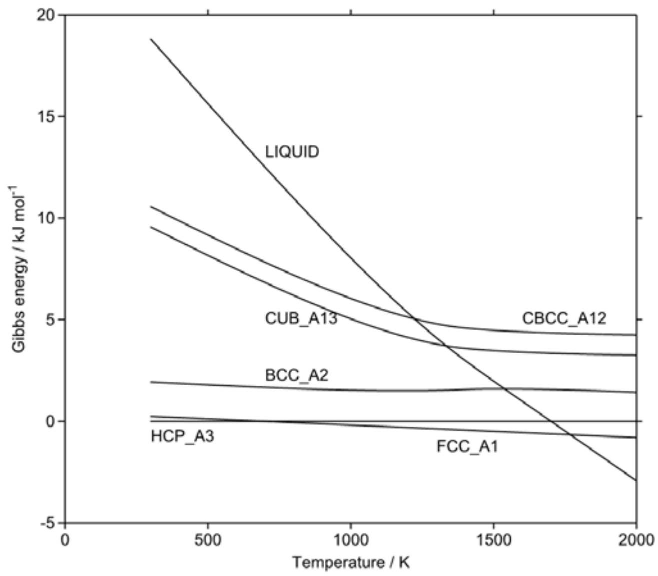
FCC_A1

$T_C = 1396$ $\quad B_0 = 1.35$
$A = 6.752927E\text{-}6$ $\quad a_0 = 3.2070159E\text{-}5$ $\quad a_1 = 5.868345E\text{-}9$
$K_0 = 4.66592E\text{-}12$ $\quad K_1 = 1.45933E\text{-}15$ $\quad K_2 = 5.17369E\text{-}20$ $\quad n = 4.007$

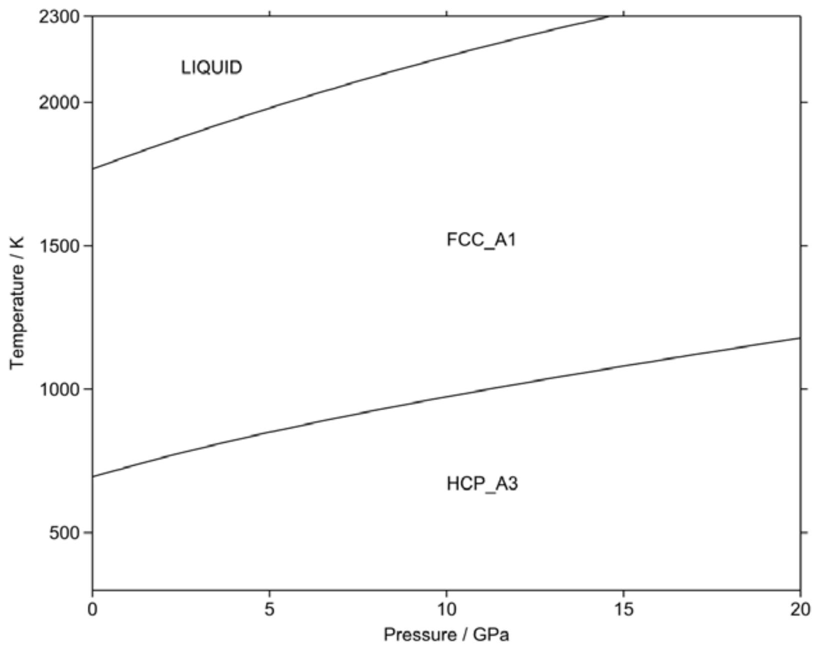
427.591 - 0.615248 T +Gpres + Gmag *(298.15 < T < 6000)*



Heat capacity of Co



Gibbs energy of phases of Co relative to HCP_A3



P-T phase diagram for Co

Cr

Source of data: *J-O Andersson, Int. J. Thermophys., 1985, 6, 411-9 [BCC_A2, LIQUID]*
J-O Andersson, A Fernandez Guillermet, P Gustafson, CALPHAD, 1987, 11, 361-4 [HCP_A3, FCC_A1]
Kaufman [CUB_A13, BCC_A12]

BCC_A2

$T_N = 311.5$ $B_0 = 0.008$
$A = 7.188E\text{-}6$ $a_0 = 1.7E\text{-}5$ $a_1 = 1.84E\text{-}8$
$K_0 = 5.2E\text{-}12$ $n = 5$

$-8856.94 + 157.48\ T - 26.908\ T \ln(T) + 1.89435E\text{-}3\ T^2 - 1.47721E\text{-}6\ T^3 + 139250\ T^{-1} + Gpres + Gmag$ *(298.15 < T < 2180)*
$-34869.344 + 344.18\ T - 50\ T \ln(T) - 2885.26E29\ T^{-9} + Gpres + Gmag$ *(2180 < T < 6000)*

LIQUID

$A = 7.188E\text{-}6$ $a_0 = 1.7E\text{-}5$ $a_1 = 1.84E\text{-}8$
$K_0 = 9.3E\text{-}12$ $n = 5$

$15483.015 + 146.059775\ T - 26.908\ T \ln(T) + 1.89435E\text{-}3\ T^2 - 1.47721E\text{-}6\ T^3 + 139250\ T^{-1}$
$+ 237.615E\text{-}23\ T^7 + Gpres$ *(298.15 < T < 2180)*
$-16459.984 + 335.616316\ T - 50\ T \ln(T) + Gpres$ *(2180 < T < 6000)*

CBCC_A12

$2230.06 + 160.1996\ T - 26.908\ T \ln(T) + 1.89435E\text{-}3\ T^2 - 1.47721E\text{-}6\ T^3 + 139250\ T^{-1}$ *(298.15 < T < 2180)*
$-23782.344 + 346.8996\ T - 50\ T \ln(T) - 2885.26E29\ T^{-9}$ *(2180 < T < 6000)*

CUB_A13

$7042.06 + 158.1076\ T - 26.908\ T \ln(T) + 1.89435E\text{-}3\ T^2 - 1.47721E\text{-}6\ T^3 + 139250\ T^{-1}$ *(298.15 < T < 2180)*
$-18970.344 + 344.8076\ T - 50\ T \ln(T) - 2885.26E29\ T^{-9}$ *(2180 < T < 6000)*

FCC_A1

$T_N = 369.667$ $B_0 = 0.82$

$-1572.94 + 157.643\ T - 26.908\ T \ln(T) + 1.89435E\text{-}3\ T^2 - 1.47721E\text{-}6\ T^3 + 139250\ T^{-1} + Gmag$ *(298.15 < T < 2180)*
$-27585.344 + 344.343\ T - 50\ T \ln(T) - 2885.26E29\ T^{-9} + Gmag$ *(2180 < T < 6000)*

HCP_A3

$T_N = 369.667$ $B_0 = 0.82$

$-4418.94 + 157.48\ T - 26.908\ T \ln(T) + 1.89435E\text{-}3\ T^2 - 1.47721E\text{-}6\ T^3 + 139250\ T^{-1} + Gmag$ *(298.15 < T < 2180)*

$-30431.344 + 344.18\ T - 50\ T \ln(T) - 2885.26E29\ T^{-9} + Gmag$ *(2180 < T < 6000)*

HCP_ZN

$-4417.94 + 157.48\ T - 26.908\ T \ln(T) + 1.89435E\text{-}3\ T^2 - 1.47721E\text{-}6\ T^3 + 139250\ T^{-1}$ *(298.15 < T < 2180)*

$-30430.344 + 344.18\ T - 50\ T \ln(T) - 2885.26E29\ T^{-9}$ *(2180 < T < 6000)*

Data relative to paramagnetic BCC_A2

BCC_A2

$T_N = 311.5$ $B_0 = 0.008$
$A = 7.188E\text{-}6$ $a_0 = 1.7E\text{-}5$ $a_1 = 1.84E\text{-}8$
$K_0 = 5.2E\text{-}12$ $n = 5$

Gmag + Gpres *(298.15 < T < 311.5)*
Gpres *(311.5 < T < 6000)*

LIQUID

$A = 7.188E\text{-}6$ $a_0 = 1.7E\text{-}5$ $a_1 = 1.84E\text{-}8$
$K_0 = 9.3E\text{-}12$ $n = 5$

$24339.955 - 11.420225\ T + 237.615E\text{-}23\ T^7 + Gpres$ *(298.15 < T < 2180)*
$18409.36 - 8.563684\ T + 2885.26E29\ T^{-9} + Gpres$ *(2180 < T < 6000)*

CBCC_A12

$11087 + 2.7196\ T$ *(298.15 < T < 6000)*

CUB_A13

$15899 + 0.6276\ T$ *(298.15 < T < 6000)*

FCC_A1

$T_N = 369.667$ $B_0 = 0.82$

$7284 + 0.163\ T + Gmag$ *(298.15 < T < 6000)*

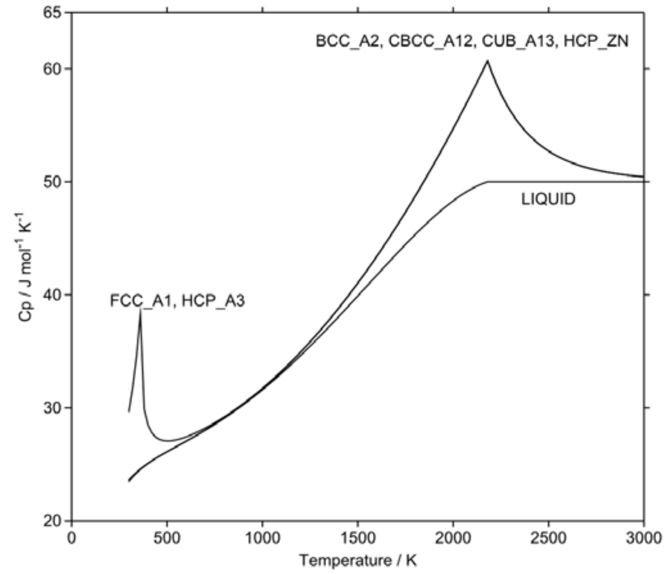
HCP_A3

$T_N = 369.667$ $\quad\quad\quad\quad$ $B_0 = 0.82$

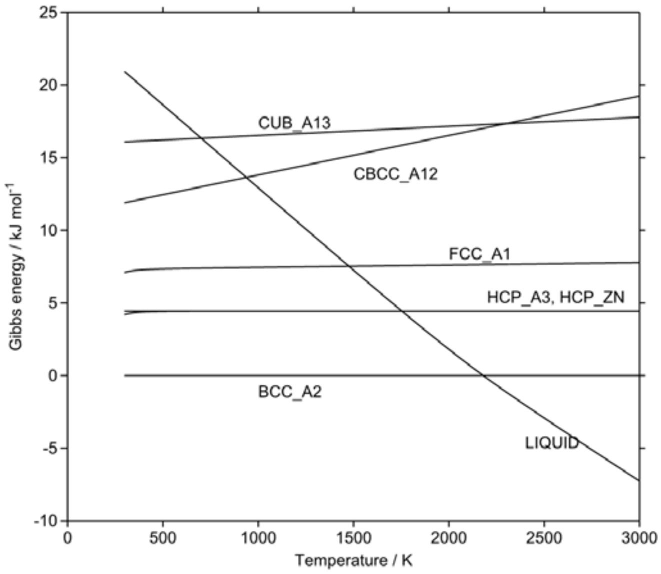
$4438 + Gmag$ *(298.15 < T < 6000)*

HCP_ZN

4439 *(298.15 < T < 6000)*



Heat capacity of Cr



Gibbs energy of phases of Cr relative to BCC_A2

Cs

Source of data: *TPIS [BCC_A2, LIQUID]*
Saunders et al. [HCP_A3, FCC_A1]

BCC_A2

$-17373.82 + 436.899787\ T - 90.5212584\ T\ln(T) + 202.9422E\text{-}3\ T^2 - 127.907669E\text{-}6\ T^3 + 245245\ T^{-1}$ *(200 < T < 301.59)*

$-13553.817 + 218.689955\ T - 46.7273304\ T\ln(T) + 20.43269E\text{-}3\ T^2 - 4.074846E\text{-}6\ T^3 + 181528\ T^{-1} + 78.016E20\ T^{-9}$ *(301.59 < T < 2000)*

LIQUID

$-15282.679 + 429.968752\ T - 90.5212584\ T\ln(T) + 202.9422E\text{-}3\ T^2 - 127.907669E\text{-}6\ T^3 + 245245\ T^{-1} - 356.867E\text{-}20\ T^7$ *(200 < T < 301.59)*

$-11454.038 + 211.728844\ T - 46.7273304\ T\ln(T) + 20.43269E\text{-}3\ T^2 - 4.074846E\text{-}6\ T^3 + 181528\ T^{-1}$ *(301.59 < T < 2000)*

FCC_A1

$-16873.82 + 438.199787\ T - 90.5212584\ T \ln(T) + 202.9422E\text{-}3\ T^2 - 127.907669E\text{-}6\ T^3 + 245245\ T^{-1}$ *(200 < T < 301.59)*

$-13053.817 + 219.989955\ T - 46.7273304\ T \ln(T) + 20.43269E\text{-}3\ T^2 - 4.074846E\text{-}6\ T^3 + 181528\ T^{-1} + 78.016E20\ T^{-9}$ *(301.59 < T < 2000)*

HCP_A3

$-16873.82 + 438.899787\ T - 90.5212584\ T \ln(T) + 202.9422E\text{-}3\ T^2 - 127.907669E\text{-}6\ T^3 + 245245\ T^{-1}$ *(200 < T < 301.59)*

$-13053.817 + 220.689955\ T - 46.7273304\ T \ln(T) + 20.43269E\text{-}3\ T^2 - 4.074846E\text{-}6\ T^3 + 181528\ T^{-1} + 78.016E20\ T^{-9}$ *(301.59 < T < 2000)*

Data relative to BCC_A2

LIQUID

$2091.141 - 6.931035\ T - 356.867E\text{-}20\ T^7$ *(200 < T < 301.59)*

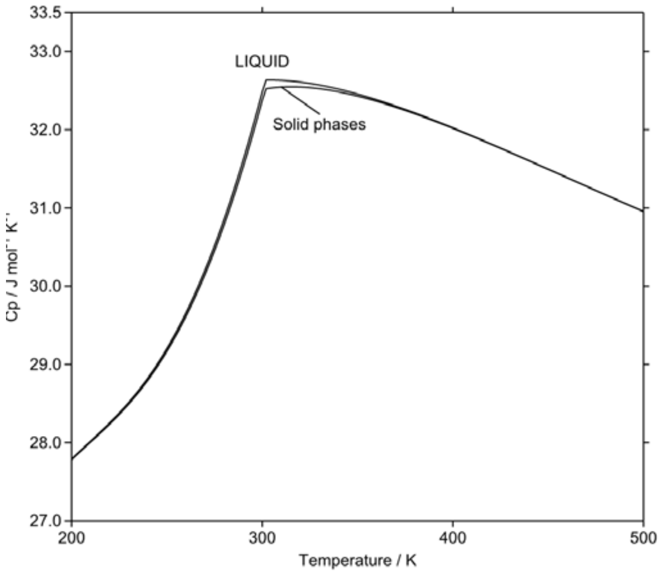
$2099.779 - 6.961111\ T - 78.016E20\ T^{-9}$ *(301.59 < T < 2000)*

FCC_A1

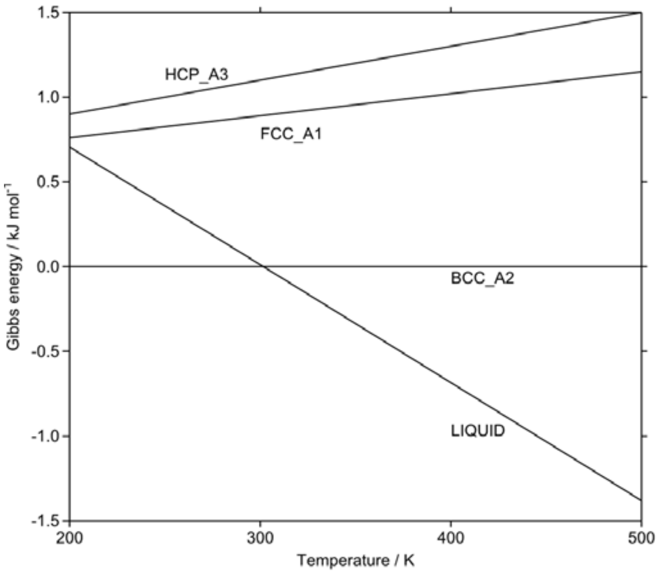
$500 + 1.3\ T$ *(200 < T < 2000)*

HCP_A3

$500 + 2\ T$ *(200 < T < 2000)*



Heat capacity of Cs



Gibbs energy of phases of Cs relative to BCC_A2

Cu

Source of data: *JANAF [FCC_A1, LIQUID]*
Saunders et al. [BCC_A2, HCP_A3]

FCC_A1

$-7770.458 + 130.485235\ T - 24.112392\ T \ln(T) - 2.65684E\text{-}3\ T^2 + 0.129223E\text{-}6\ T^3 + 52478\ T^{-1}$
(298.15 < T < 1357.77)
$-13542.026 + 183.803828\ T - 31.38\ T \ln(T) + 364.167E27\ T^{-9}$ *(1357.77 < T < 3200)*

LIQUID

$5194.277 + 120.973331\ T - 24.112392\ T \ln(T) - 2.65684E\text{-}3\ T^2 + 0.129223E\text{-}6\ T^3$
$+ 52478\ T^{-1} - 584.89E\text{-}23\ T^7$ *(298.15 < T < 1357.77)*
$-46.545 + 173.881484\ T - 31.38\ T \ln(T)$ *(1357.77 < T < 3200)*

BCC_A2

$-3753.458 + 129.230235\ T - 24.112392\ T \ln(T) - 2.65684E\text{-}3\ T^2 + 0.129223E\text{-}6\ T^3 + 52478\ T^{-1}$
(298.15 < T < 1357.77)
$-9525.026 + 182.548828\ T - 31.38\ T \ln(T) + 364.167E27\ T^{-9}$ *(1357.77 < T < 3200)*

HCP_A3

$-7170.458 + 130.685235\ T - 24.112392\ T \ln(T) - 2.65684E\text{-}3\ T^2 + 0.129223E\text{-}6\ T^3 + 52478\ T^{-1}$
(298.15 < T < 1357.77)
$-12942.026 + 184.003828\ T - 31.38\ T \ln(T) + 364.167E27\ T^{-9}$ *(1357.77 < T < 3200)*

HCP_ZN

$-7170.458 + 130.685235\ T - 24.112392\ T \ln(T) - 2.65684E\text{-}3\ T^2 + 0.129223E\text{-}6\ T^3 + 52478\ T^{-1}$
(298.15 < T < 1357.77)
$-12942.026 + 184.003828\ T - 31.38\ T \ln(T) + 364.167E27\ T^{-9}$ *(1357.77 < T < 3200)*

Data relative to FCC_A1

LIQUID

$12964.735 - 9.511904\ T - 584.89E\text{-}23\ T^7$ *(298.15 < T < 1357.77)*
$13495.481 - 9.922344\ T - 364.167E27\ T^{-9}$ *(1357.77 < T < 3200)*

BCC_A2

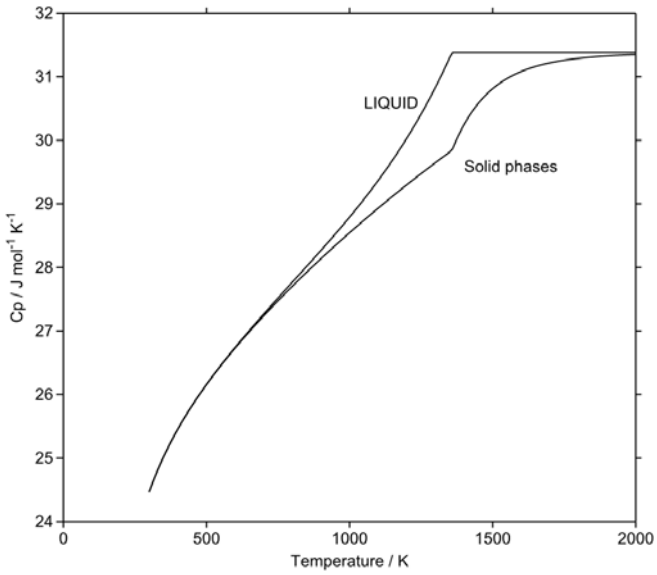
$4017 - 1.255\ T$ *(298.15 < T < 3200)*

HCP_A3

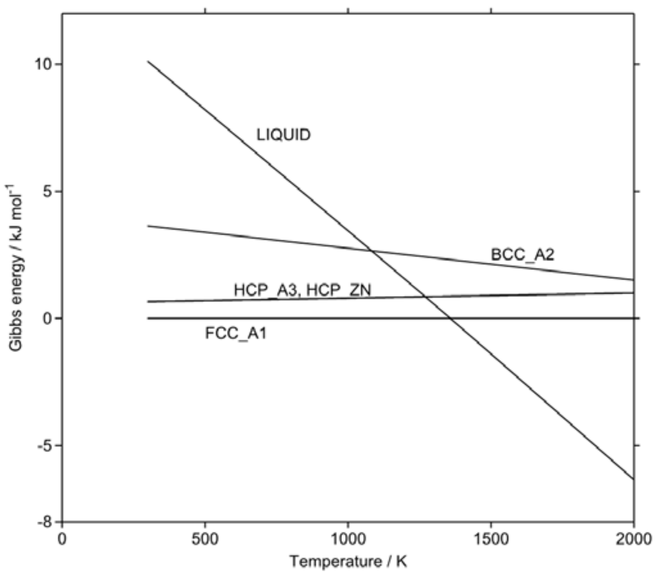
600 + 0.2 T *(298.15 < T < 3200)*

HCP_ZN

600 + 0.2 T *(298.15 < T < 3200)*



Heat capacity of Cu



Gibbs energy of phases of Cu relative to FCC_A1

Dy

Source of data: *Huasen Shen, Weijing Zhang, Guoquan Liu, Run Wang and Zhenmin Du, Report F-95-01, May 1995, University of Science and Technology, Beijing [HCP_A3, BCC_A2, LIQUID]*

HCP_A3

$T_C = 179.0$ $B_0 = 3.0$

$-7937.166 + 102.307412\ T - 26.3917167\ T \ln(T) - 0.761684E\text{-}3\ T^2 - 0.586914E\text{-}6\ T^3 + 4011\ T^{-1} + Gmag$ *(100 < T < 1000)*

$-13733.328 + 214.012934\ T - 43.8283359\ T \ln(T) + 16.69098E\text{-}3\ T^2 - 3.497028E\text{-}6\ T^3 + Gmag$ *(1000 < T < 1654.15)*

$-404681.371 + 2032.1415\ T - 272.123952\ T \ln(T) + 57.830168E\text{-}3\ T^2 - 2.761691E\text{-}6\ T^3 + 109616238\ T^{-1} + Gmag$ *(1654.15 < T < 3000)*

BCC_A2

$-6428.986 + 101.740796\ T - 26.3917167\ T \ln(T) - 0.761684E\text{-}3\ T^2 - 0.586914E\text{-}6\ T^3 + 4011\ T^{-1}$ *(100 < T < 1000)*

$327500.062 - 2868.04585\ T + 391.515418\ T\ ln(T) - 224.042148E{-3}\ T^2 + 20.407608E{-6}\ T^3$
$- 48652656\ T^{-1}$ *(1000 < T < 1654.15)*
$-33708.795 + 291.409631\ T - 50.208\ T\ ln(T)$ *(1654.15 < T < 1685.15)*
$-40775.497 + 330.318068\ T - 55.2811171\ T\ ln(T) + 1.525467E{-3}\ T^2 - 0.077437E{-6}\ T^3 + 1776589\ T^{-1}$
(1685.15 < T < 3000)

LIQUID

$5259.453 + 94.763048\ T - 26.3917167\ T\ ln(T) - 0.761684E{-3}\ T^2 - 0.586914E{-6}\ T^3 + 4011\ T^{-1}$
(100 < T < 1000)
$300126.971 - 2519.78614\ T + 341.302578\ T\ ln(T) - 196.153225E{-3}\ T^2 + 17.61978E{-6}\ T^3 - 43071677\ T^{-1}$
(1000 < T < 1685.15)
$-21864.734 + 282.205014\ T - 49.9151\ T\ ln(T)$ *(1685.15 < T < 3000)*

Data relative to paramagnetic HCP_A3

HCP_A3

$T_C = 179.0$ $B_0 = 3.0$

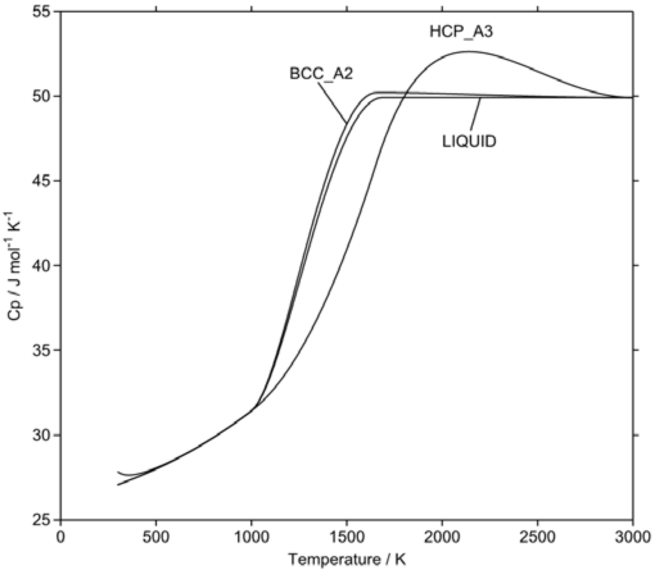
Gmag *(1685.15 < T < 3000)*

BCC_A2

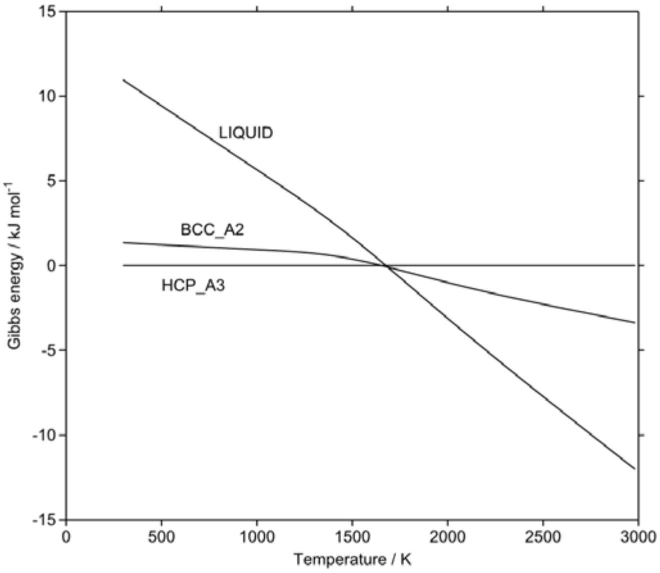
$1508.18 - 0.566616\ T$ *(100 < T < 1000)*
$341233.39 - 3082.058784\ T + 435.3437539\ T\ ln(T) - 240.733128E{-3}\ T^2 + 23.904636E{-6}\ T^3$
$- 48652657\ T^{-1}$ *(1000 < T < 1654.15)*
$370972.576 - 1740.731869\ T + 221.915952\ T\ ln(T) - 57.830168E{-3}\ T^2 + 2.761691E{-6}\ T^3$
$- 109616238\ T^{-1}$ *(1654.15 < T < 1685.15)*
$363905.874 - 1701.823432\ T + 216.8428349\ T\ ln(T) - 56.304701E{-3}\ T^2 + 2.684254E{-6}\ T^3$
$- 107839649\ T^{-1}$ *(1685.15 < T < 3000)*

LIQUID

$13196.619 - 7.544364\ T$ *(100 < T < 1000)*
$313860.299 - 2733.799074\ T + 385.1309139\ T\ ln(T) - 212.844205E{-3}\ T^2 + 21.116808E{-6}\ T^3$
$- 43071678\ T^{-1}$ *(1000 < T < 1654.15)*
$704808.342 - 4551.92764\ T + 613.42653\ T\ ln(T) - 253.983393E{-3}\ T^2 + 20.381471E{-6}\ T^3$
$- 152687915\ T^{-1}$ *(1654.15 < T < 1685.15)*
$382816.637 - 1749.936486\ T + 222.208852\ T\ ln(T) - 57.830168E{-3}\ T^2 + 2.761691E{-6}\ T^3$
$- 109616238\ T^{-1}$ *(1685.15 < T < 3000)*



Heat capacity of Dy



Gibbs energy of phases of Dy relative to HCP_A3

Er

Source of data: *Hultgren [HCP_A3, LIQUID]*
S Norgren, J Phase Equil.; 2000, 21(2), 148-156 [BCC_A2]

HCP_A3

$-8489.136 + 116.698964\ T - 28.3846744\ T\ln(T) + 0.995792\text{E-}3\ T^2 - 0.952557\text{E-}6\ T^3 + 9581\ T^{-1}$ *(298.15 < T < 1802)*

$-445688.206 + 2233.102116\ T - 298.1351305\ T\ln(T) + 65.950553\text{E-}3\ T^2 - 3.041405\text{E-}6\ T^3 + 123973199\ T^{-1}$ *(1802 < T < 3200)*

LIQUID

$10892.966 + 106.457118\ T - 28.3846744\ T\ln(T) + 0.995792\text{E-}3\ T^2 - 0.952557\text{E-}6\ T^3 + 9581\ T^{-1}$ *(298.15 < T < 500)*

$17912.678 + 0.355564\ T - 12.0761776\ T\ln(T) - 14.414687\text{E-}3\ T^2 + 1.316517\text{E-}6\ T^3 - 528122\ T^{-1}$ *(500 < T < 1802)*

$747.131 + 187.623024\ T - 38.702\ T\ln(T)$ *(1802 < T < 3200)*

BCC_A2

$-3889.136 + 114.204611\ T - 28.3846744\ T\ln(T) + 0.995792\text{E-}3\ T^2 - 0.952557\text{E-}6\ T^3 + 9581\ T^{-1}$ *(298.15 < T < 1802)*

$-441088.206 + 2230.607763\ T - 298.1351305\ T\ln(T) + 65.950553\text{E-}3\ T^2 - 3.041405\text{E-}6\ T^3 + 123973199\ T^{-1}$ *(1802 < T < 3200)*

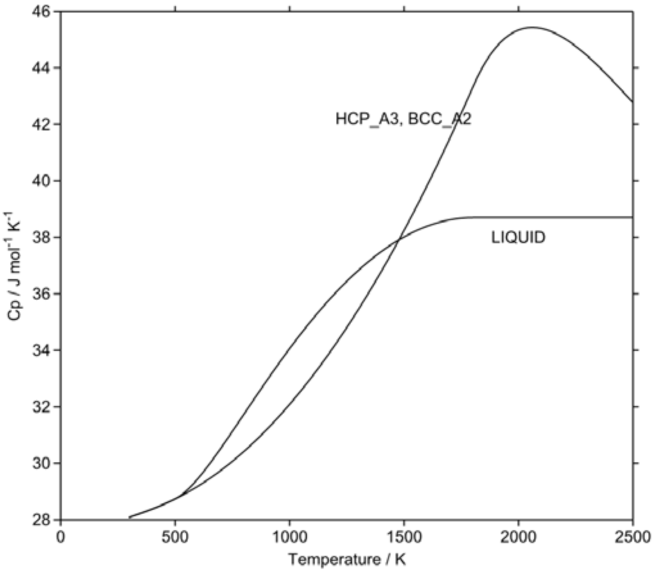
Data relative to HCP_A3

LIQUID

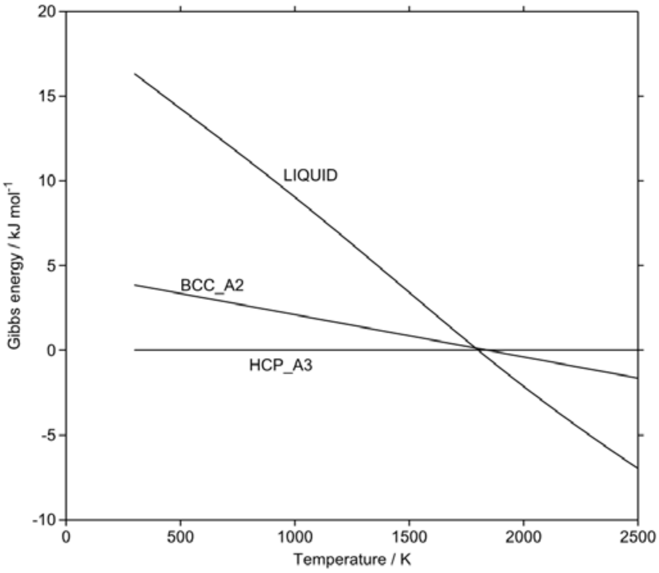
$19382.102 - 10.241846\ T$ *(298.15 < T < 500)*
$26401.814 - 116.3434\ T + 16.3084968\ T\ \ln(T) - 15.410479E\text{-}3\ T^{2} + 2.269074E\text{-}6\ T^{3} - 537703\ T^{-1}$
(500 < T < 1802)
$446435.337 - 2045.479092\ T + 259.4331305\ T\ \ln(T) - 65.950553E\text{-}3\ T^{2} + 3.041405E\text{-}6\ T^{3}$
$- 123973199\ T^{-1}$ *(1802 < T < 3200)*

BCC_A2

$4600 - 2.494353\ T$ *(298.15 < T < 3200)*



Heat capacity of Er



Gibbs energy of phases of Er relative to HCP_A3

Eu

Source of data: *Hultgren [BCC_A2, LIQUID]*

BCC_A2

$-9864.965 + 135.836737\ T - 32.8418896\ T\ \ln(T) + 9.31735E\text{-}3\ T^{2} - 4.006564E\text{-}6\ T^{3} + 102717\ T^{-1}$
(298.15 < T < 1095)
$-287423.476 + 2174.733036\ T - 309.3571009\ T\ \ln(T) + 114.530917E\text{-}3\ T^{2} - 8.809866E\text{-}6\ T^{3}$
$+ 48455305\ T^{-1}$ *(1095 < T < 1900)*
$-13663.125 + 182.113799\ T - 38.11624\ T\ \ln(T)$ *(1900 < T < 1901)*

LIQUID

$-1482.46 + 128.661522\ T - 32.8418896\ T\ \ln(T) + 9.31735E\text{-}3\ T^2 - 4.006564E\text{-}6\ T^3 + 102717\ T^{-1}$ *(298.15 < T < 400)*

$10972.726 - 103.688201\ T + 4.3501554\ T\ \ln(T) - 36.811218E\text{-}3\ T^2 + 5.452934E\text{-}6\ T^3 - 646908\ T^{-1}$ *(400 < T < 1095)*

$-6890.641 + 175.517247\ T - 38.11624\ T\ \ln(T)$ *(1095 < T < 1900)*

Data relative to BCC_A2

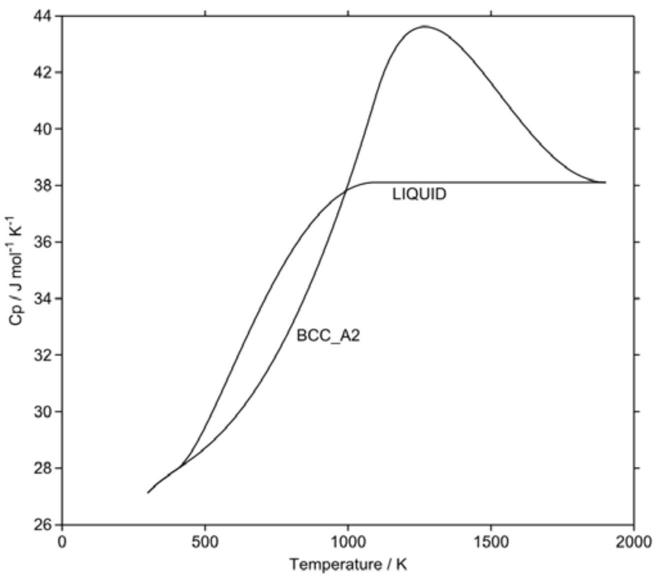
LIQUID

$8382.505 - 7.175215\ T$ *(298.15 < T < 400)*

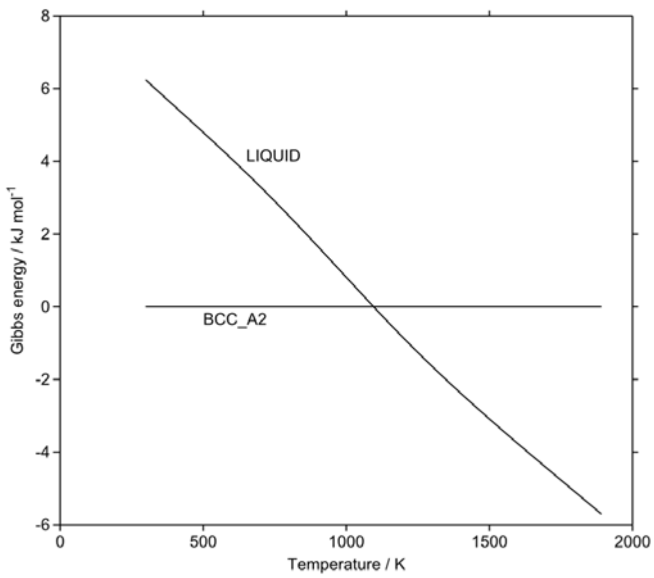
$20837.691 - 239.524938\ T + 37.192045\ T\ \ln(T) - 46.128568E\text{-}3\ T^2 + 9.459498E\text{-}6\ T^3 - 749625\ T^{-1}$ *(400 < T < 1095)*

$280532.835 - 1999.215789\ T + 271.2408609\ T\ \ln(T) - 114.530917E\text{-}3\ T^2 + 8.809866E\text{-}6\ T^3 - 48455305\ T^{-1}$ *(1095 < T < 1900)*

$6772.484 - 6.596552\ T$ *(1900 < T < 1901)*



Heat capacity of Eu



Gibbs energy of phases of Eu relative to BCC_A2

Fe

Source of data: *A Fernandez Guillermet, P Gustafson, High Temp. - High Press., 1985,* ***16****, 591-610. [BCC_A2, LIQUID]*
A Fernandez Guillermet, P Gustafson, High Temp. - High Press., 1985, ***16****, 591-610. modified slightly for high temperature range [FCC_A1, HCP_A3]*
Weiming Huang, TRITA-MAC-0388 [BCC_A12, CUB_A13]

BCC_A2

$T_C = 1043$ $B_0 = 2.22$
$A = 7.042095E-6$ $a_0 = 2.3987E-5$ $a_1 = 2.569E-8$
$K_0 = 5.965E-12$ $K_1 = 6.5152E-17$ $n = 4.7041$

$1225.7 + 124.134\ T - 23.5143\ T \ln(T) - 4.39752E-3\ T^2 - 0.058927E-6\ T^3 + 77359\ T^{-1}$ +Gpres + Gmag *(298.15 < T < 1811)*
$-25383.581 + 299.31255\ T - 46\ T \ln(T) + 2296.03E28\ T^{-9}$ +Gpres + Gmag *(1811 < T < 6000)*

FCC_A1

$T_N = 67$ $B_0 = 0.7$
$A = 6.688726E-6$ $a_0 = 7.3097E-5$
$K_0 = 6.2951E-12$ $K_1 = 6.5152E-17$ $n = 5.1665$

$-236.7 + 132.416\ T - 24.6643\ T \ln(T) - 3.75752E-3\ T^2 - 0.058927E-6\ T^3 + 77359\ T^{-1}$ +Gpres + Gmag *(298.15 < T < 1811)*
$-27097.396 + 300.252559\ T - 46\ T \ln(T) + 2788.54E28\ T^{-9}$ +Gpres + Gmag *(1811 < T < 6000)*

LIQUID

$A = 6.62574E-6$ $a_0 = 10.7895E-5$ $a_3 = -25.79493$
$K_0 = 0.75475E-12$ $K_1 = 485.09E-17$ $n = 6.59834$

$13265.87 + 117.57557\ T - 23.5143\ T \ln(T) - 4.39752E-3\ T^2 - 0.058927E-6\ T^3 + 77359\ T^{-1}$
$- 367.516E-23\ T^7$ +Gpres *(298.15 < T < 1811)*
$-10838.83 + 291.302\ T - 46\ T \ln(T)$ +Gpres *(1811 < T < 6000)*

HCP_A3

$A = 6.59121E-6$ $a_0 = 7.3646E-5$
$K_0 = 6.2951E-12$ $K_1 = 6.5152E-17$ $n = 5.1665$

$-2480.08 + 136.725\ T - 24.6643\ T \ln(T) - 3.75752E-3\ T^2 - 0.058927E-6\ T^3 + 77359\ T^{-1}$ +Gpres *(298.15 < T < 1811)*
$-29340.776 + 304.561559\ T - 46\ T \ln(T) + 2788.54E28\ T^{-9}$ +Gpres *(1811 < T < 6000)*

ORTHORHOMBIC_A20

$6225.7 + 124.134\ T - 23.5143\ T \ln(T) - 4.39752E-3\ T^2 - 0.058927E-6\ T^3 + 77359\ T^{-1}$ *(298.15 < T < 1811)*

$-20383.581 + 299.31255\,T - 46\,T\ln(T) + 2296.03E28\,T^{-9}$ *(1811 < T < 6000)*

TETRAGONAL_U

$6225.7 + 124.134\,T - 23.5143\,T\ln(T) - 4.39752E{-3}\,T^2 - 0.058927E{-6}\,T^3 + 77359\,T^{-1}$
(298.15 < T < 1811)
$-20383.581 + 299.31255\,T - 46\,T\ln(T) + 2296.03E28\,T^{-9}$ *(1811 < T < 6000)*

CBCC_A12

$5970.7 + 124.134\,T - 23.5143\,T\ln(T) - 4.39752E{-3}\,T^2 - 0.058927E{-6}\,T^3 + 77359\,T^{-1}$
(298.15 < T < 1811)
$-20638.581 + 299.31255\,T - 46\,T\ln(T) + 2296.03E28\,T^{-9}$ *(1811 < T < 6000)*

CUB_A13

$4970.7 + 124.134\,T - 23.5143\,T\ln(T) - 4.39752E{-3}\,T^2 - 0.058927E{-6}\,T^3 + 77359\,T^{-1}$
(298.15 < T < 1811)
$-21638.581 + 299.31255\,T - 46\,T\ln(T) + 2296.03E28\,T^{-9}$ *(1811 < T < 6000)*

Data relative to paramagnetic BCC_A2

BCC_A2

$T_C = 1043$	$B_0 = 2.22$	
$A = 7.042095E{-6}$	$a_0 = 2.3987E{-5}$	$a_1 = 2.569E{-8}$
$K_0 = 5.965E{-12}$	$K_1 = 6.5152E{-17}$	$n = 4.7041$

Gmag + Gpres *(298.15 < T < 6000)*

FCC_A1

$T_N = 67$	$B_0 = 0.7$	
$A = 6.688726E{-6}$	$a_0 = 7.3097E{-5}$	
$K_0 = 6.2951E{-12}$	$K_1 = 6.5152E{-17}$	$n = 5.1665$

$-1462.4 + 8.282\,T - 1.15\,T\ln(T) + 0.64E{-3}\,T^2$ +Gpres + Gmag *(298.15 < T < 1811)*
$-1713.815 + 0.940009\,T + 492.51E28\,T^{-9}$ +Gpres + Gmag *(1811 < T < 6000)*

LIQUID

$A = 6.62574E{-6}$	$a_0 = 10.7895E{-5}$	$a_3 = -25.79493$
$K_0 = 0.75475E{-12}$	$K_1 = 485.09E{-17}$	$n = 6.59834$

$12040.17 - 6.55843\,T - 367.516E{-23}\,T^7$ +Gpres *(298.15 < T < 1811)*
$14544.751 - 8.01055\,T - 2296.03E28\,T^{-9}$ +Gpres *(1811 < T < 6000)*

HCP_A3

A = 6.59121E-6 a_0 = 7.3646E-5
K_0 = 6.2951E-12 K_1 = 6.5152E-17 n = 5.1665

-3705.78 + 12.591 T - 1.15 T ln(T) + 0.64E-3 T^2 +Gpres *(298.15 < T < 1811)*
-3957.195 + 5.249009 T + 492.51E28 T^{-9} +Gpres *(1811 < T < 6000)*

ORTHORHOMBIC_A20

5000 *(298.15 < T < 6000)*

TETRAGONAL_U

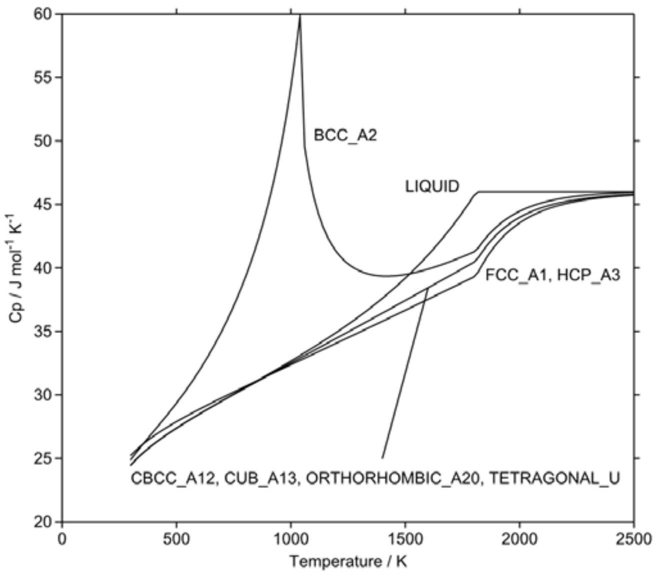
5000 *(298.15 < T < 6000)*

CBCC_A12

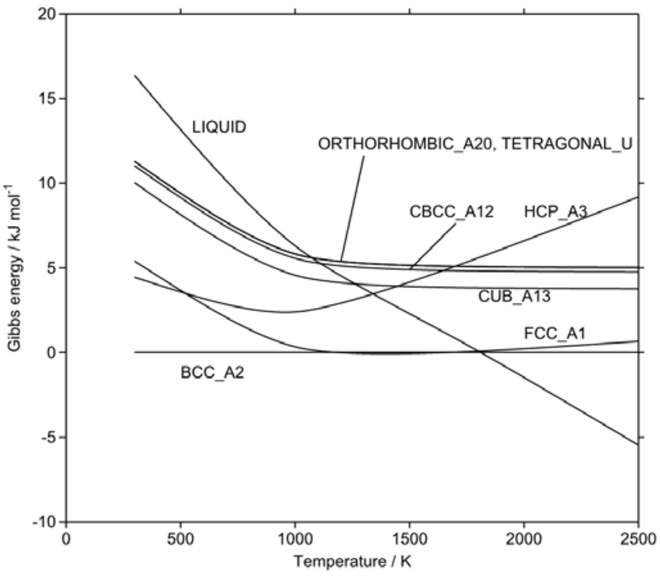
4745 *(298.15 < T < 6000)*

CUB_A13

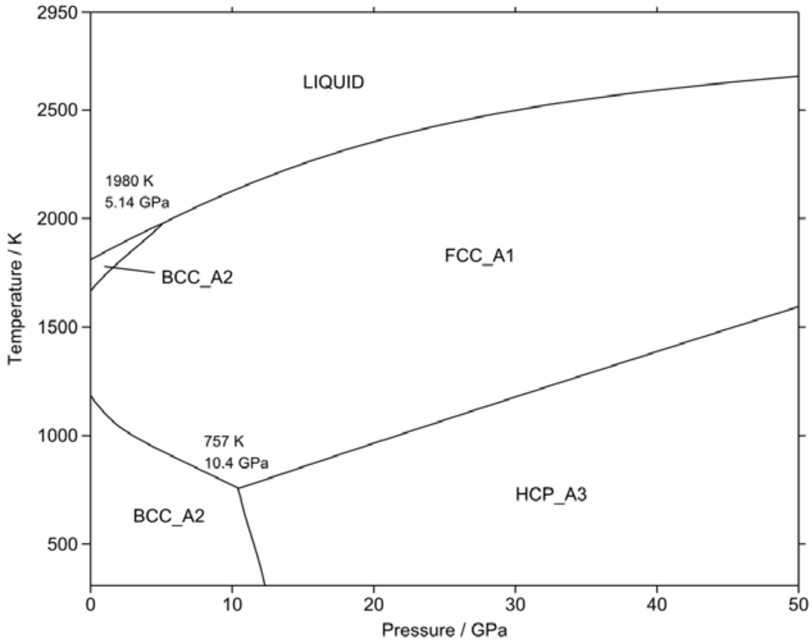
3745 *(298.15 < T < 6000)*



Heat capacity of Fe



Gibbs energy of phases of Fe relative to BCC_A2



P-T phase diagram for Fe

Ga

Source of data : *TPIS [ORTHORHOMBIC, LIQUID]*
I Ansara (unpublished work) [BCT_A5]
Saunders et al. [FCC_A1, HCP_A3, BCC_A2, TET_A6]
P Franke, unpublished [DIAMOND_A4]

ORTHORHOMBIC_GA

$-21312.331 + 585.263691\ T - 108.2287832\ T\ \ln(T) + 227.155636E{-3}\ T^2 - 118.575257E{-6}\ T^3 + 439954\ T^{-1}$ *(200 < T < 302.91)*

$-7055.643 + 132.73019\ T - 26.0692906\ T\ \ln(T) + 0.1506E{-3}\ T^2 - 0.040173E{-6}\ T^3 - 118332\ T^{-1} + 164.547E21\ T^{-9}$ *(302.91 < T < 4000)*

LIQUID

$-15821.033 + 567.189696\ T - 108.2287832\ T\ \ln(T) + 227.155636E{-3}\ T^2 - 118.575257E{-6}\ T^3 + 439954\ T^{-1} - 70.171E{-18}\ T^7$ *(200 < T < 302.91)*

$-1389.188 + 114.049043\ T - 26.0692906\ T\ \ln(T) + 0.1506E{-3}\ T^2 - 0.040173E{-6}\ T^3 - 118332\ T^{-1}$ *(302.91 < T < 4000)*

BCT_A5

$-17466.331 + 575.463691\ T - 108.2287832\ T\ \ln(T) + 227.155636E{-3}\ T^2 - 118.575257E{-6}\ T^3 + 439954\ T^{-1}$ *(200 < T < 302.91)*

$-3209.643 + 122.93019\ T - 26.0692906\ T\ \ln(T) + 0.1506E{-3}\ T^2 - 0.040173E{-6}\ T^3 - 118332\ T^{-1} + 164.547E21\ T^{-9}$ *(302.91 < T < 4000)*

TETRAGONAL_A6

$-17812.331 + 575.263691\ T - 108.2287832\ T\ \ln(T) + 227.155636E{-3}\ T^2 - 118.575257E{-6}\ T^3$
$+ 439954\ T^{-1}$ *(200 < T < 302.91)*
$-3555.643 + 122.73019\ T - 26.0692906\ T\ \ln(T) + 0.1506E{-3}\ T^2 - 0.040173E{-6}\ T^3 - 118332\ T^{-1}$
$+ 164.547E21\ T^{-9}$ *(302.91 < T < 4000)*

BCC_A2

$-16812.331 + 573.563691\ T - 108.2287832\ T\ \ln(T) + 227.155636E{-3}\ T^2 - 118.575257E{-6}\ T^3$
$+ 439954\ T^{-1}$ *(200 < T < 302.91)*
$-2555.643 + 121.03019\ T - 26.0692906\ T\ \ln(T) + 0.1506E{-3}\ T^2 - 0.040173E{-6}\ T^3 - 118332\ T^{-1}$
$+ 164.547E21\ T^{-9}$ *(302.91 < T < 4000)*

FCC_A1

$-17512.331 + 575.063691\ T - 108.2287832\ T\ \ln(T) + 227.155636E{-3}\ T^2 - 118.575257E{-6}\ T^3$
$+ 439954\ T^{-1}$ *(200 < T < 302.91)*
$-3255.643 + 122.53019\ T - 26.0692906\ T\ \ln(T) + 0.1506E{-3}\ T^2 - 0.040173E{-6}\ T^3 - 118332\ T^{-1}$
$+ 164.547E21\ T^{-9}$ *(302.91 < T < 4000)*

HCP_A3

$-16812.331 + 575.763691\ T - 108.2287832\ T\ \ln(T) + 227.155636E{-3}\ T^2 - 118.575257E{-6}\ T^3$
$+ 439954\ T^{-1}$ *(200 < T < 302.91)*
$-2555.643 + 123.23019\ T - 26.0692906\ T\ \ln(T) + 0.1506E{-3}\ T^2 - 0.040173E{-6}\ T^3 - 118332\ T^{-1}$
$+ 164.547E21\ T^{-9}$ *(302.91 < T < 4000)*

HCP_ZN

$-16811.331 + 575.763691\ T - 108.2287832\ T\ \ln(T) + 227.155636E{-3}\ T^2 - 118.575257E{-6}\ T^3$
$+ 439954\ T^{-1}$ *(200 < T < 302.91)*
$-2554.643 + 123.23019\ T - 26.0692906\ T\ \ln(T) + 0.1506E{-3}\ T^2 - 0.040173E{-6}\ T^3 - 118332\ T^{-1}$
$+ 164.547E21\ T^{-9}$ *(302.91 < T < 4000)*

DIAMOND_A4

$-412.331 + 583.263691\ T - 108.2287832\ T\ \ln(T) + 227.155636E{-3}\ T^2 - 118.575257E{-6}\ T^3 + 439954\ T^{-1}$
(200 < T < 302.91)
$13844.357 + 130.73019\ T - 26.0692906\ T\ \ln(T) + 0.1506E{-3}\ T^2 - 0.040173E{-6}\ T^3 - 118332\ T^{-1}$
$+ 164.547E21\ T^{-9}$ *(302.91 < T < 4000)*

Data relative to ORTHORHOMBIC_GA

LIQUID

$5491.298 - 18.073995\ T - 70.171E\text{-}18\ T^{7}$ *(200 < T < 302.91)*
$5666.455 - 18.681147\ T - 164.547E21\ T^{-9}$ *(302.91 < T < 4000)*

BCT_A5

3846 - 9.8 T *(200 < T < 4000)*

TETRAGONAL_A6

3500 - 10 T *(200 < T < 4000)*

BCC_A2

4500 - 11.7 T *(200 < T < 4000)*

FCC_A1

3800 - 10.2 T *(200 < T < 4000)*

HCP_A3

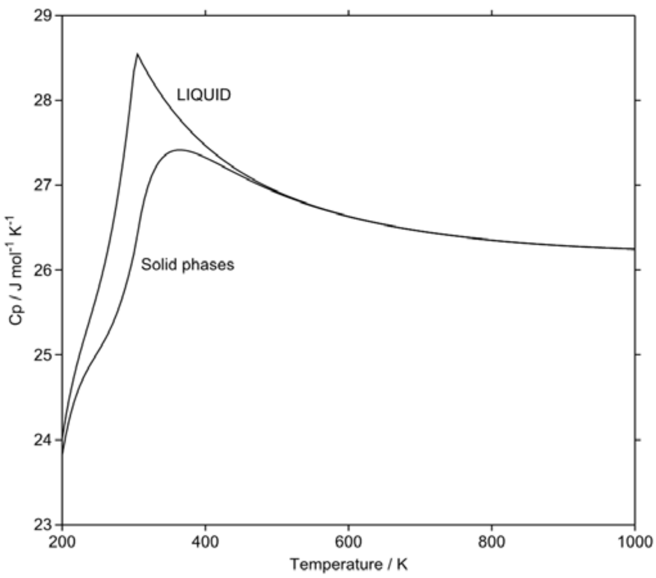
4500 - 9.5 T *(200 < T < 4000)*

HCP_ZN

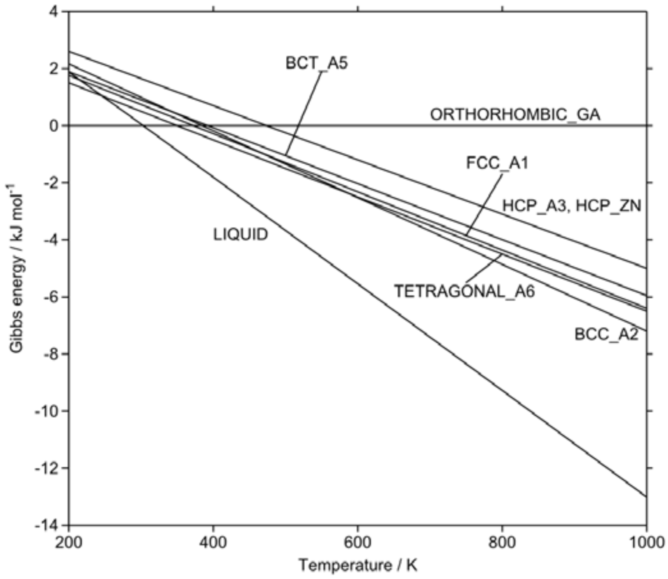
4501 - 9.5 T *(200 < T < 4000)*

DIAMOND_A4

20900 - 2 T *(200 < T < 4000)*



Heat capacity of Ga



Gibbs energy of phases of Ga relative to ORTHORHOMBIC_GA

Gd

Source of data: *Huasen Shen, Weijing Zhang, Guoquan Liu, Run Wang and Zhenmin Du; Report F-95-02, May 1995, University of Science and Technology, Beijing [HCP_A3, BCC_A2 and LIQUID]*
M Zinkevich, N Mattern, H J Seiffert; J. Phase Equil.; 2000, 21(4), 385-394 [FCC_A1]

HCP_A3

$T_C = 293.40$ $B_0 = 3.0$

$-6834.585 + 97.13101\ T - 24.7214131\ T\ln(T) - 2.852405E-3\ T^2 - 0.314674E-6\ T^3 - 8666\ T^{-1} + Gmag$
(200 < T < 1000)
$-6483.254 + 95.691992\ T - 24.6598297\ T\ln(T) - 1.85225E-3\ T^2 - 0.661212E-6\ T^3 + Gmag$
(1000 < T < 1508.15)
$-123124.992 + 699.125537\ T - 101.800197\ T\ln(T) + 15.064425E-3\ T^2 - 0.639166E-6\ T^3 + 29356890\ T^{-1} + Gmag$
(1508.15 < T < 3600)

BCC_A2

$-3600.777 + 95.019164\ T - 24.721413\ T\ln(T) - 2.852405E-3\ T^2 - 0.314674E-6\ T^3 - 8666\ T^{-1}$
(100 < T < 1000)
$152792.743 - 1349.58873\ T + 180.097094\ T\ln(T) - 119.550229E-3\ T^2 + 11.791573E-6\ T^3 - 22038836\ T^{-1}$
(1000 < T < 1508.15)
$-15783.762 + 202.222183\ T - 38.960425\ T\ln(T)$ *(1508.15 < T < 1586.15)*
$-19850.556 + 224.818035\ T - 41.904333\ T\ln(T) + 0.858223E-3\ T^2 - 0.037757E-6\ T^3 + 995429\ T^{-1}$
(1586.15 < T < 3600)

LIQUID

$6225.441 + 88.80921\ T - 24.7214131\ T\ln(T) - 2.852405E\text{-}3\ T^2 - 0.314674E\text{-}6\ T^3 - 8666\ T^{-1}$

(100 < T < 1000)

$146262.037 - 1208.70685\ T + 159.352082\ T\ln(T) - 108.247135E\text{-}3\ T^2 + 10.694551E\text{-}6\ T^3 - 19678357\ T^{-1}$ *(1000 < T < 1508.15)*

$-5397.314 + 192.336215\ T - 38.5075\ T\ln(T)$ *(1508.15 < T < 3600)*

FCC_A1

$-6334.585 + 97.13101\ T - 24.7214131\ T\ln(T) - 2.852405E\text{-}3\ T^2 - 0.314674E\text{-}6\ T^3 - 8666\ T^{-1}$

(200 < T < 1000)

$-5983.254 + 95.691992\ T - 24.6598297\ T\ln(T) - 1.85225E\text{-}3\ T^2 - 0.661212E\text{-}6\ T^3$ *(1000 < T < 1508.15)*

$-122624.992 + 699.125537\ T - 101.800197\ T\ln(T) + 15.064425E\text{-}3\ T^2 - 0.639166E\text{-}6\ T^3 + 29356890\ T^{-1}$

(1508.15 < T < 3600)

Data relative to paramagnetic HCP_A3

HCP_A3

$T_C = 293.40$ $B_0 = 3.0$

Gmag

BCC_A2

$3233.809 - 2.111846\ T$ *(200 < T < 1000)*

$159275.997 - 1445.280722\ T + 204.7569237\ T\ln(T) - 117.697979E\text{-}3\ T^2 + 12.452784E\text{-}6\ T^3 - 22038836\ T^{-1}$ *(1000 < T < 1508.15)*

$107341.23 - 496.90348\ T + 62.839772\ T\ln(T) - 15.064425E\text{-}3\ T^2 + 0.639166E\text{-}6\ T^3 - 29356890\ T^{-1}$

(1508.15 < T < 1586.15)

$103274.436 - 474.307628\ T + 59.895864\ T\ln(T) - 14.206202E\text{-}3\ T^2 + 0.601409E\text{-}6\ T^3 - 28361462\ T^{-1}$

(1586.15 < T < 3600)

LIQUID

$13060.026 - 8.3218\ T$ *(200 < T < 1000)*

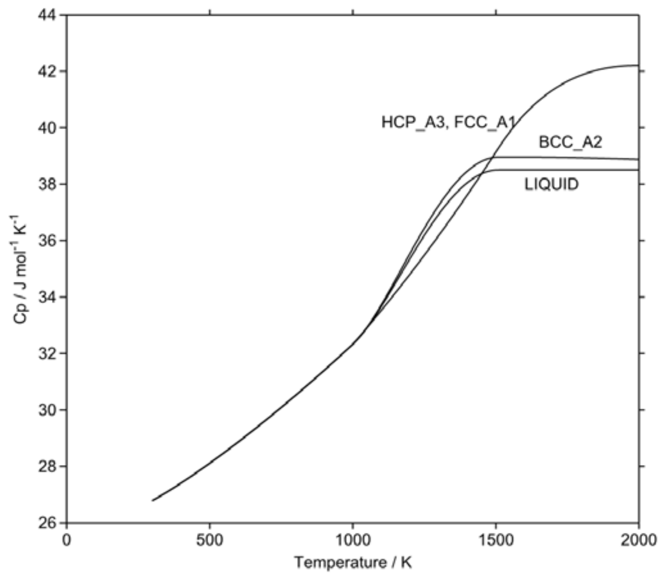
$152745.291 - 1304.398842\ T + 184.0119117\ T\ln(T) - 106.394885E\text{-}3\ T^2 + 11.355762E\text{-}6\ T^3 - 19678357\ T^{-1}$ *(1000 < T < 1508.15)*

$117727.678 - 506.789322\ T + 63.292697\ T\ln(T) - 15.064425E\text{-}3\ T^2 + 0.639166E\text{-}6\ T^3 - 29356890\ T^{-1}$

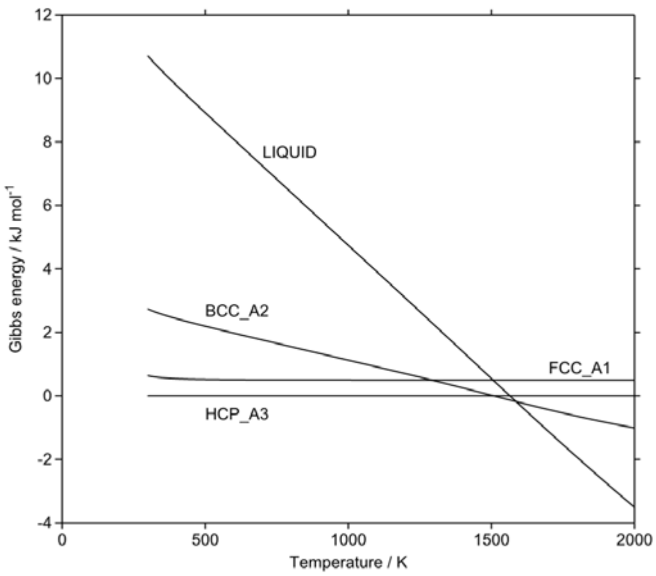
(1508.15 < T < 3600)

FCC_A1

500 *(200 < T < 3600)*



Heat capacity of Gd



Gibbs energy of phases of Gd relative to HCP_A3

Ge

Source of data: *Hultgren [DIAMOND_A4, LIQUID]*
Saunders et al. [FCC_A1, BCC_A2, HCP_A3]
A T Dinsdale (unpublished) [BCT_A5, RHOMBOHEDRAL_A7]

DIAMOND_A4

$-9486.153 + 165.635573\,T - 29.5337682\,T\ln(T) + 5.568297E{-}3\,T^2 - 1.513694E{-}6\,T^3 + 163298\,T^{-1}$ $(298.15 < T < 900)$

$-5689.239 + 102.86087\,T - 19.8536239\,T\ln(T) - 3.672527E{-}3\,T^2$ $(900 < T < 1211.4)$

$-9548.204 + 156.708024\,T - 27.6144\,T\ln(T) - 859.809E26\,T^{-9}$ $(1211.4 < T < 3200)$

LIQUID

$27655.337 + 134.94853\,T - 29.5337682\,T\ln(T) + 5.568297E{-}3\,T^2 - 1.513694E{-}6\,T^3 + 163298\,T^{-1} + 856.632E{-}23\,T^7$ $(298.15 < T < 900)$

$31452.25 + 72.173826\,T - 19.8536239\,T\ln(T) - 3.672527E{-}3\,T^2 + 856.632E{-}23\,T^7$ $(900 < T < 1211.4)$

$27243.473 + 126.324186\,T - 27.6144\,T\ln(T)$ $(1211.4 < T < 3200)$

BCT_A5

$19313.847 + 149.135573\,T - 29.5337682\,T\ln(T) + 5.568297E{-}3\,T^2 - 1.513694E{-}6\,T^3 + 163298\,T^{-1}$ $(298.15 < T < 900)$

$23110.761 + 86.36087\,T - 19.8536239\,T\ln(T) - 3.672527E{-}3\,T^2$ $(900 < T < 1211.4)$

$19251.796 + 140.208024\,T - 27.6144\,T\ln(T) - 859.809E26\,T^{-9}$ $(1211.4 < T < 3000)$

RHOMBOHEDRAL_A7

$20313.847 + 149.135573\ T - 29.5337682\ T\ln(T) + 5.568297E\text{-}3\ T^2 - 1.513694E\text{-}6\ T^3 + 163298\ T^{-1}$ *(298.15 < T < 900)*
$24110.761 + 86.36087\ T - 19.8536239\ T\ln(T) - 3.672527E\text{-}3\ T^2$ *(900 < T < 1211.4)*
$20251.796 + 140.208024\ T - 27.6144\ T\ln(T) - 859.809E26\ T^{-9}$ *(1211.4 < T < 3000)*

BCC_A2

$24613.847 + 142.135573\ T - 29.5337682\ T\ln(T) + 5.568297E\text{-}3\ T^2 - 1.513694E\text{-}6\ T^3 + 163298\ T^{-1}$ *(298.15 < T < 900)*
$28410.761 + 79.36087\ T - 19.8536239\ T\ln(T) - 3.672527E\text{-}3\ T^2$ *(900 < T < 1211.4)*
$24551.796 + 133.208024\ T - 27.6144\ T\ln(T) - 859.809E26\ T^{-9}$ *(1211.4 < T < 3200)*

FCC_A1

$26513.847 + 143.335573\ T - 29.5337682\ T\ln(T) + 5.568297E\text{-}3\ T^2 - 1.513694E\text{-}6\ T^3 + 163298\ T^{-1}$ *(298.15 < T < 900)*
$30310.761 + 80.56087\ T - 19.8536239\ T\ln(T) - 3.672527E\text{-}3\ T^2$ *(900 < T < 1211.4)*
$26451.796 + 134.408024\ T - 27.6144\ T\ln(T) - 859.809E26\ T^{-9}$ *(1211.4 < T < 3200)*

HCP_A3

$25513.847 + 144.135573\ T - 29.5337682\ T\ln(T) + 5.568297E\text{-}3\ T^2 - 1.513694E\text{-}6\ T^3 + 163298\ T^{-1}$ *(298.15 < T < 900)*
$29310.761 + 81.36087\ T - 19.8536239\ T\ln(T) - 3.672527E\text{-}3\ T^2$ *(900 < T < 1211.4)*
$25451.796 + 135.208024\ T - 27.6144\ T\ln(T) - 859.809E26\ T^{-9}$ *(1211.4 < T < 3200)*

Data relative to DIAMOND_A4

LIQUID

$37141.489 - 30.687043\ T + 856.632E\text{-}23\ T^7$ *(298.15 < T < 1211.4)*
$36791.677 - 30.383838\ T + 859.809E26\ T^{-9}$ *(1211.4 < T < 3200)*

BCT_A5

$28800 - 16.5\ T$ *(298.15 < T < 3000)*

RHOMBOHEDRAL_A7

$29800 - 16.5\ T$ *(298.15 < T < 3000)*

BCC_A2

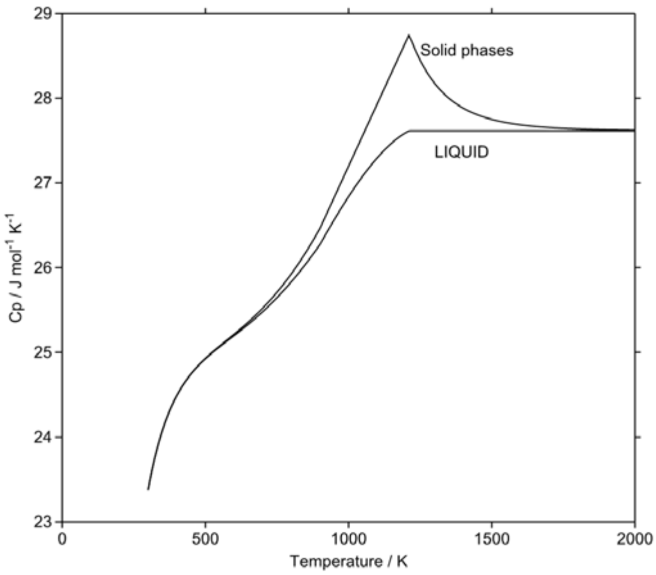
$34100 - 23.5\ T$ *(298.15 < T < 3200)*

FCC_A1

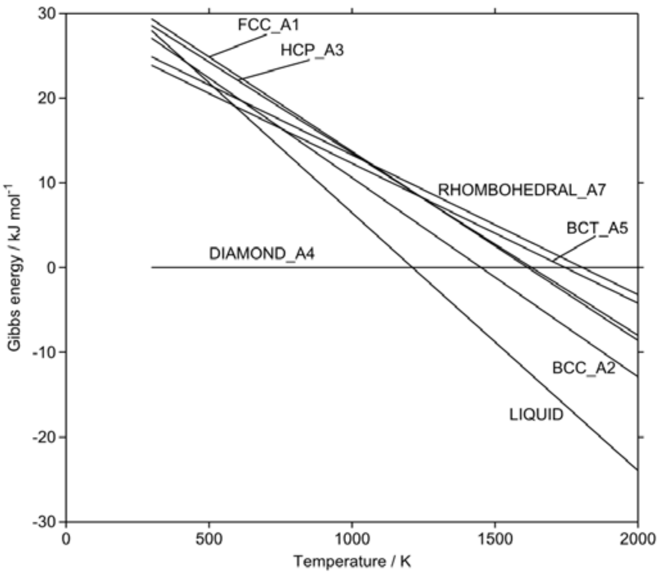
$36000 - 22.3\ T$ *(298.15 < T < 3200)*

HCP_A3

$35000 - 21.5\ T$ *(298.15 < T < 3200)*



Heat capacity of Ge



Gibbs energy of phases of Ge relative to DIAMOND_A4

Hf

Source of data: *N Saunders, A T Dinsdale (Unpublished work)*

HCP_A3

$-6987.297 + 110.744026\ T - 22.7075\ T \ln(T) - 4.146145E{-3}\ T^2 - 0.000477E{-6}\ T^3 - 22590\ T^{-1}$ *(298.15 < T < 2506)*

$-1446776.329 + 6193.609991\ T - 787.5363829\ T \ln(T) + 173.5215E{-3}\ T^2 - 7.575759E{-6}\ T^3 + 501742495\ T^{-1}$ *(2506 < T < 3000)*

$-34274.698 + 277.882368\ T - 44\ T \ln(T)$ *(3000 < T < 3001)*

BCC_A2

$5370.703 + 103.836026\ T - 22.8995\ T \ln(T) - 4.206605E{-3}\ T^2 + 0.871923E{-6}\ T^3 - 22590\ T^{-1} - 0.1446E{-9}\ T^4$ *(298.15 < T < 2506)*

$1912456.771 - 8624.20573\ T + 1087.6141247\ T \ln(T) - 286.857065E{-3}\ T^2 + 13.427829E{-6}\ T^3 - 610085091\ T^{-1}$ *(2506 < T < 3000)*

$-32498.178 + 276.723247\ T - 44\ T \ln(T)$ *(3000 < T < 3001)*

LIQUID

$20414.959 + 99.790933\ T - 22.7075\ T\ \ln(T) - 4.146145E\text{-}3\ T^2 - 0.000477E\text{-}6\ T^3 - 22590\ T^{-1}$
(298.15 < T < 1000)
$49731.499 - 149.91739\ T + 12.116812\ T\ \ln(T) - 21.262021E\text{-}3\ T^2 + 1.376466E\text{-}6\ T^3 - 4449699\ T^{-1}$
(1000 < T < 2506)
$-4247.217 + 265.470523\ T - 44\ T\ \ln(T)$ *(2506 < T < 3001)*

FCC_A1

$3012.703 + 108.544026\ T - 22.7075\ T\ \ln(T) - 4.146145E\text{-}3\ T^2 - 0.000477E\text{-}6\ T^3 - 22590\ T^{-1}$
(298.15 < T < 2506)
$-1436776.329 + 6191.409991\ T - 787.5363829\ T\ \ln(T) + 173.5215E\text{-}3\ T^2 - 7.575759E\text{-}6\ T^3$
$+ 501742495\ T^{-1}$ *(2506 < T < 3000)*
$-24274.698 + 275.682368\ T - 44\ T\ \ln(T)$ *(3000 < T < 3001)*

Data relative to HCP_A3

BCC_A2

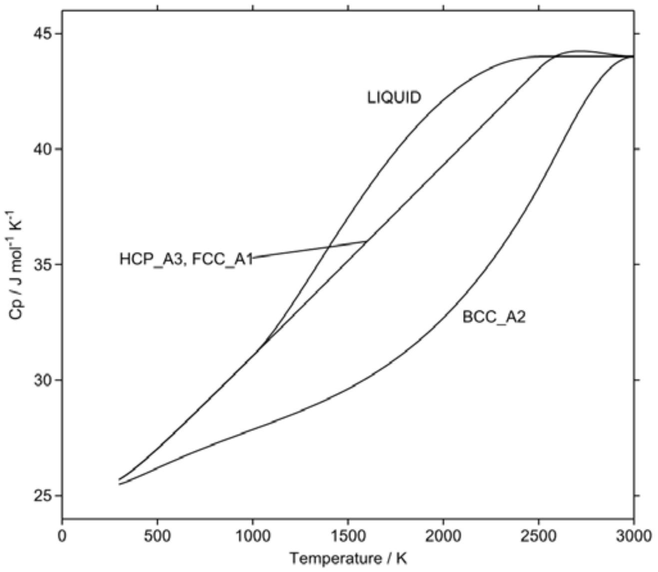
$12358 - 6.908\ T - 0.192\ T\ \ln(T) - 0.06046E\text{-}3\ T^2 + 0.8724E\text{-}6\ T^3 - 0.1446E\text{-}9\ T4$ *(298.15 < T < 2506)*
$3359233.1 - 14817.815721\ T + 1875.1505076\ T\ \ln(T) - 460.378565E\text{-}3\ T^2 + 21.003588E\text{-}6\ T^3$
$- 1111827586\ T^{-1}$ *(2506 < T < 3000)*
$1776.52 - 1.159121\ T$ *(3000 < T < 3001)*

LIQUID

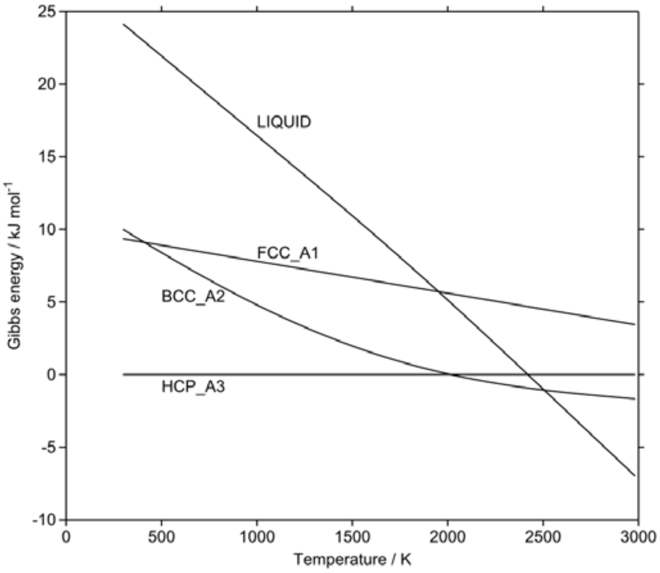
$27402.256 - 10.953093\ T$ *(298.15 < T < 1000)*
$56718.796 - 260.661416\ T + 34.824312\ T\ \ln(T) - 17.115876E\text{-}3\ T^2 + 1.376943E\text{-}6\ T^3 - 4427109\ T^{-1}$
(1000 < T < 2506)
$1442529.112 - 5928.139468\ T + 743.5363829\ T\ \ln(T) - 173.5215E\text{-}3\ T^2 + 7.575759E\text{-}6\ T^3$
$- 501742495\ T^{-1}$ *(2506 < T < 3000)*
$30027.481 - 12.411845\ T$ *(3000 < T < 3001)*

FCC_A1

$10000 - 2.2\ T$ *(298.15 < T < 3001)*



Heat capacity of Hf



Gibbs energy of phases of Hf relative to HCP_A3

Hg

Source of data: *Hultgren [RHOMBO_A10, LIQUID]*
J Jang,N J Silk, A Watson, A W Bryant, T G Chart, B B Argent, CALPHAD, 1995, 19(3), 415 [RHOMBO_A10, HCP_A3]
A Maitre; J M Fiorani, M Vilasi, J Phase Equilib; 2002, 23(4), 329 [FCC_A1]

LIQUID

$82356.855 - 3348.194658\,T + 618.1933082\,T\ln(T) - 2028.2337\text{E-}3\,T^2 + 1183.982129\text{E-}6\,T^3 - 2366612\,T^{-1}$ *(200 < T < 234.32)*

$-8961.207 + 135.232291\,T - 32.257\,T\ln(T) + 9.7977\text{E-}3\,T^2 - 3.20695\text{E-}6\,T^3 + 6670\,T^{-1}$ *(234.32 < T < 400)*

$-7970.627 + 112.33345\,T - 28.414\,T\ln(T) + 3.18535\text{E-}3\,T^2 - 1.077802\text{E-}6\,T^3 - 41095\,T^{-1}$ *(400 < T < 700)*

$-7161.338 + 90.797305\,T - 24.87\,T\ln(T) - 1.66775\text{E-}3\,T^2 + 0.008737\text{E-}6\,T^3 - 27495\,T^{-1}$ *(700 < T < 2000)*

RHOMBO_A10

$-10668.401 + 123.274598\,T - 28.847\,T\ln(T) + 16.99705\text{E-}3\,T^2 - 24.555667\text{E-}6\,T^3 + 13330\,T^{-1}$ *(200 < T < 234.32)*

$-11425.394 + 135.928158\,T - 30.2091\,T\ln(T) + 1.07555\text{E-}3\,T^2 - 0.228298\text{E-}6\,T^3 + 35545\,T^{-1}$ *(234.32 < T < 2000)*

TETRAGONAL_A6

$-10459.721 + 125.04019\,T - 28.847\,T\ln(T) + 16.99705\text{E-}3\,T^2 - 24.555667\text{E-}6\,T^3 + 13330\,T^{-1}$ *(200 < T < 234.32)*

$-11216.714 + 137.69375\ T - 30.2091\ T\ln(T) + 1.07555E\text{-}3\ T^2 - 0.228298E\text{-}6\ T^3 + 35545\ T^{-1}$
(234.32 < T < 2000)

HCP_A3

$-10468.401 + 123.974598\ T - 28.847\ T\ln(T) + 16.99705E\text{-}3\ T^2 - 24.555667E\text{-}6\ T^3 + 13330\ T^{-1}$
(200 < T < 234.32)
$-11225.394 + 136.628158\ T - 30.2091\ T\ln(T) + 1.07555E\text{-}3\ T^2 - 0.228298E\text{-}6\ T^3 + 35545\ T^{-1}$
(234.32 < T < 2000)

FCC_A1

$82361.855 - 3339.826658\ T + 618.1933082\ T\ln(T) - 2028.2337E\text{-}3\ T^2 + 1183.982129E\text{-}6\ T^3 - 2366612\ T^{-1}$
(200 < T < 234.32)
$-8956.207 + 143.600291\ T - 32.257\ T\ln(T) + 9.7977E\text{-}3\ T^2 - 3.20695E\text{-}6\ T^3 + 6670\ T^{-1}$
(234.32 < T < 400)
$-7965.627 + 120.70145\ T - 28.414\ T\ln(T) + 3.18535E\text{-}3\ T^2 - 1.077802E\text{-}6\ T^3 - 41095\ T^{-1}$
(400 < T < 700)
$-7156.338 + 99.165305\ T - 24.87\ T\ln(T) - 1.66775E\text{-}3\ T^2 + 0.008737E\text{-}6\ T^3 - 27495\ T^{-1}$
(700 < T < 2000)

Data relative to LIQUID

RHOMBO_A10

$-93025.256 + 3471.469256\ T - 647.0403082\ T\ln(T) + 2045.23075E\text{-}3\ T^2 - 1208.537796E\text{-}6\ T^3 + 2379942\ T^{-1}$
(200 < T < 234.32)
$-2464.187 + 0.695867\ T + 2.0479\ T\ln(T) - 8.72215E\text{-}3\ T^2 + 2.978652E\text{-}6\ T^3 + 28875\ T^{-1}$
(234.32 < T < 400)
$-3454.767 + 23.594708\ T - 1.7951\ T\ln(T) - 2.1098E\text{-}3\ T^2 + 0.849504E\text{-}6\ T^3 + 76640\ T^{-1}$
(400 < T < 700)
$-4264.056 + 45.130853\ T - 5.3391\ T\ln(T) + 2.7433E\text{-}3\ T^2 - 0.237035E\text{-}6\ T^3 + 63040\ T^{-1}$
(700 < T < 2000)

TETRAGONAL_A6

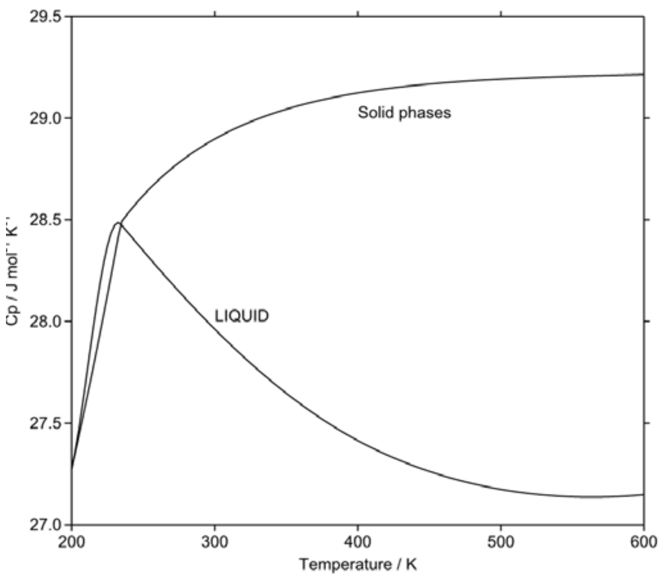
$-92816.576 + 3473.234848\ T - 647.0403082\ T\ln(T) + 2045.23075E\text{-}3\ T^2 - 1208.537796E\text{-}6\ T^3 + 2379942\ T^{-1}$
(200 < T < 234.32)
$-2255.507 + 2.461459\ T + 2.0479\ T\ln(T) - 8.72215E\text{-}3\ T^2 + 2.978652E\text{-}6\ T^3 + 28875\ T^{-1}$
(234.32 < T < 400)
$-3246.087 + 25.3603\ T - 1.7951\ T\ln(T) - 2.1098E\text{-}3\ T^2 + 0.849504E\text{-}6\ T^3 + 76640\ T^{-1}$
(400 < T < 700)
$-4055.376 + 46.896445\ T - 5.3391\ T\ln(T) + 2.7433E\text{-}3\ T^2 - 0.237035E\text{-}6\ T^3 + 63040\ T^{-1}$
(700 < T < 2000)

HCP_A3

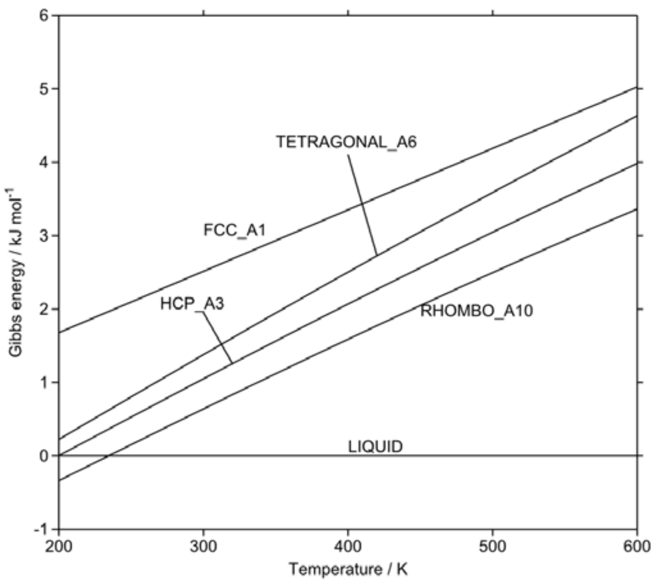
$-92825.256 + 3472.169256\ T - 647.0403082\ T \ln(T) + 2045.23075E\text{-}3\ T^2 - 1208.537796E\text{-}6\ T^3$
$+ 2379942\ T^{-1}$ *(200 < T < 234.32)*
$-2264.187 + 1.395867\ T + 2.0479\ T \ln(T) - 8.72215E\text{-}3\ T^2 + 2.978652E\text{-}6\ T^3 + 28875\ T^{-1}$
(234.32 < T < 400)
$-3254.767 + 24.294708\ T - 1.7951\ T \ln(T) - 2.1098E\text{-}3\ T^2 + 0.849504E\text{-}6\ T^3 + 76640\ T^{-1}$
(400 < T < 700)
$-4064.056 + 45.830853\ T - 5.3391\ T \ln(T) + 2.7433E\text{-}3\ T^2 - 0.237035E\text{-}6\ T^3 + 63040\ T^{-1}$
(700 < T < 2000)

FCC_A1

$5 + 8.368\ T$ *(200 < T < 2000)*



Heat capacity of Hg



Gibbs energy of phases of Hg relative to LIQUID

Ho

Source of data: *Hultgren, modified by M H Rand and A T Dinsdale [HCP_A3]*
S Norgren; J. Phase Equil., 2000, 21(2), 148-156 [BCC_A2, LIQUID]

HCP_A3

$-7612.429 + 86.593171\ T - 23.4879\ T \ln(T) - 8.27315E\text{-}3\ T^2 + 2.375467E\text{-}6\ T^3$ *(298.15 < T < 600)*
$-10917.688 + 182.475691\ T - 39.6932\ T \ln(T) + 18.20065E\text{-}3\ T^2 - 4.829733E\text{-}6\ T^3$ *(600 < T < 900)*
$46646.188 - 421.474473\ T + 48.0595\ T \ln(T) - 42.4634E\text{-}3\ T^2 + 3.233133E\text{-}6\ T^3 - 7185900\ T^{-1}$
(900 < T < 1200)
$27786.061 - 156.162846\ T + 8.28608\ T \ln(T) - 10.82725E\text{-}3\ T^2 - 1.112352E\text{-}6\ T^3 - 6183850\ T^{-1}$
(1200 < T < 1703)

$-825364.662 + 4248.379056\,T - 558.9506818\,T\ln(T) + 139.111904E\text{-}3\,T^2 - 6.824652E\text{-}6\,T^3 + 219952973\,T^{-1}$ *(1703 < T < 3000)*

$-17149.229 + 235.898104\,T - 43.932\,T\ln(T)$ *(3000 < T < 3001)*

LIQUID

$9770.993 + 76.600977\,T - 23.4879\,T\ln(T) - 8.27315E\text{-}3\,T^2 + 2.375467E\text{-}6\,T^3$ *(298.15 < T < 600)*

$6465.734 + 172.483497\,T - 39.6932\,T\ln(T) + 18.20065E\text{-}3\,T^2 - 4.829733E\text{-}6\,T^3$ *(600 < T < 900)*

$64029.25 - 431.466667\,T + 48.0595\,T\ln(T) - 42.4634E\text{-}3\,T^2 + 3.233133E\text{-}6\,T^3 - 7185900\,T^{-1}$ *(900 < T < 1000)*

$124827.533 - 994.683024\,T + 127.9577778\,T\ln(T) - 88.196514E\text{-}3\,T^2 + 8.008222E\text{-}6\,T^3 - 15727191\,T^{-1}$ *(1000 < T < 1703)*

$-9688.531 + 230.793918\,T - 43.932\,T\ln(T)$ *(1703 < T < 3001)*

BCC_A2

$-3773.06 + 84.546902\,T - 23.4879\,T\ln(T) - 8.27315E\text{-}3\,T^2 + 2.375467E\text{-}6\,T^3$ *(298.15 < T < 600)*

$-7078.318 + 180.429422\,T - 39.6932\,T\ln(T) + 18.20065E\text{-}3\,T^2 - 4.829733E\text{-}6\,T^3$ *(600 < T < 900)*

$50485.557 - 423.520743\,T + 48.0595\,T\ln(T) - 42.4634E\text{-}3\,T^2 + 3.233133E\text{-}6\,T^3 - 7185900\,T^{-1}$ *(900 < T < 1000)*

$185620.196 - 1635.726622\,T + 218.9372486\,T\ln(T) - 135.16576E\text{-}3\,T^2 + 12.168911E\text{-}6\,T^3 - 26729747\,T^{-1}$ *(1000 < T < 1703)*

$-28759.761 + 272.961035\,T - 48.116\,T\ln(T)$ *(1703 < T < 1745)*

$-152646.008 + 939.778244\,T - 134.7930638\,T\ln(T) + 25.544089E\text{-}3\,T^2 - 1.287517E\text{-}6\,T^3 + 32050889\,T^{-1}$ *(1745 < T < 3000)*

$-19066.44 + 236.390471\,T - 43.932\,T\ln(T)$ *(3000 < T < 3001)*

Data relative to HCP_A3

LIQUID

$17383.422 - 9.992194\,T$ *(298.15 < T < 1000)*

$78181.345 - 573.208551\,T + 79.8982778\,T\ln(T) - 45.733114E\text{-}3\,T^2 + 4.775089E\text{-}6\,T^3 - 8541291\,T^{-1}$ *(1000 < T < 1200)*

$97041.472 - 838.520178\,T + 119.6716978\,T\ln(T) - 77.369264E\text{-}3\,T^2 + 9.120574E\text{-}6\,T^3 - 9543341\,T^{-1}$ *(1200 < T < 1703)*

$815676.131 - 4017.585138\,T + 515.0186818\,T\ln(T) - 139.111904E\text{-}3\,T^2 + 6.824652E\text{-}6\,T^3 - 219952973\,T^{-1}$ *(1703 < T < 3000)*

$7460.698 - 5.104186\,T$ *(3000 < T < 3001)*

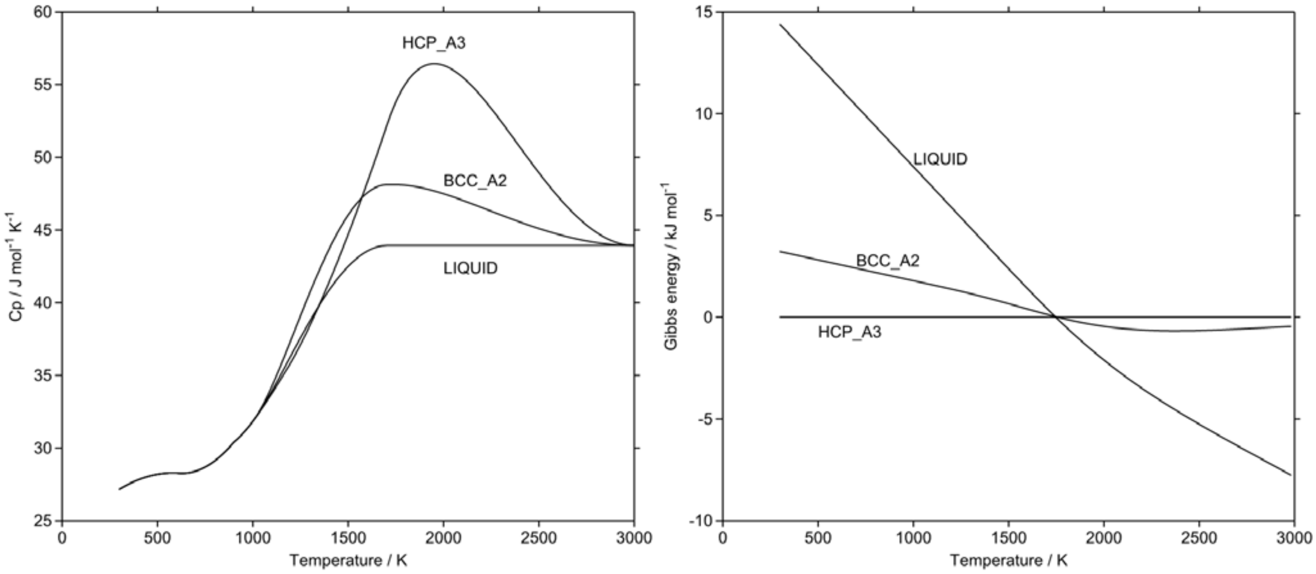
BCC_A2

$3839.369 - 2.046269\,T$ *(298.15 < T < 1000)*

$138974.008 - 1214.252149\,T + 170.8777486\,T\ln(T) - 92.70236E\text{-}3\,T^2 + 8.935778E\text{-}6\,T^3 - 19543847\,T^{-1}$ *(1000 < T < 1200)*

$157834.135 - 1479.563776\,T + 210.6511686\,T\ln(T) - 124.33851E\text{-}3\,T^2 + 13.281263E\text{-}6\,T^3 - 20545897\,T^{-1}$ *(1200 < T < 1703)*

$796604.901 - 3975.418021 T + 510.8346818 T \ln(T) - 139.111904E{-3} T^2 + 6.824652E{-6} T^3$
$- 219952973 T^{-1}$ *(1703 < T < 1745)*
$672718.654 - 3308.600812 T + 424.157618 T \ln(T) - 113.567815E{-3} T^2 + 5.537135E{-6} T^3$
$- 187902084 T^{-1}$ *(1745 < T < 3000)*
$-1917.211 + 0.492367 T$ *(3000 < T < 3001)*



Heat capacity of Ho   Gibbs energy of phases of Ho relative to HCP_A3

In

Source of data: *TPIS [TETRAGONAL_A6, LIQUID]*
I Ansara, Unpublished work, 1989 [HCP_A3]
D Boa, I Ansara, Thermochimica Acta 1998, 314, 79-86 [FCC_A1, RHOMBOHEDRAL_A7]
Saunders et al. [BCC_A2]
J P Nabot, I Ansara, Bull. Alloy Phase Diag., 1987, ***8****, 246 [TET_ALPHA1]*
H S Liu, Y Cui, K Ishida, Z P Jin, CALPHAD, 2003, 27, 27-37 [DHCP]

TETRAGONAL_A6

$-6978.89 + 92.338115 T - 21.8386 T \ln(T) - 5.72566E{-3} T^2 - 2.120321E{-6} T^3 - 22906 T^{-1}$
(298.15 < T < 429.7485)
$-7033.514 + 124.476588 T - 27.4562 T \ln(T) + 0.54607E{-3} T^2 - 0.08367E{-6} T^3 - 211708 T^{-1}$
$+ 353.332E20 T^{-9}$ *(429.7485 < T < 3800)*

LIQUID

$-3696.799 + 84.70123 T - 21.8386 T \ln(T) - 5.72566E{-3} T^2 - 2.120321E{-6} T^3 - 22906 T^{-1}$
$- 559.405E{-22} T^7$ *(298.15 < T < 429.7485)*
$-3749.808 + 116.835756 T - 27.4562 T \ln(T) + 0.54607E{-3} T^2 - 0.08367E{-6} T^3 - 211708 T^{-1}$
(429.7485 < T < 3800)

BCT_A5

$-1938.02 + 88.998425\ T - 21.8386\ T\ln(T) - 5.72566E\text{-}3\ T^2 - 2.120321E\text{-}6\ T^3 - 22906\ T^{-1}$

(298.15 < T < 429.7485)

$-1992.644 + 121.136898\ T - 27.4562\ T\ln(T) + 0.54607E\text{-}3\ T^2 - 0.08367E\text{-}6\ T^3 - 211708\ T^{-1} + 353.332E20\ T^{-9}$

(429.7485 < T < 3000)

RHOMBOHEDRAL_A7

$-2794.89 + 92.338115\ T - 21.8386\ T\ln(T) - 5.72566E\text{-}3\ T^2 - 2.120321E\text{-}6\ T^3 - 22906\ T^{-1}$

(298.15 < T < 429.7485)

$-2849.514 + 124.476588\ T - 27.4562\ T\ln(T) + 0.54607E\text{-}3\ T^2 - 0.08367E\text{-}6\ T^3 - 211708\ T^{-1} + 353.332E20\ T^{-9}$

(429.7485 < T < 3000)

TET_ALPHA1

$-6855.89 + 92.139315\ T - 21.8386\ T\ln(T) - 5.72566E\text{-}3\ T^2 - 2.120321E\text{-}6\ T^3 - 22906\ T^{-1}$

(298.15 < T < 429.7485)

$-6910.514 + 124.277788\ T - 27.4562\ T\ln(T) + 0.54607E\text{-}3\ T^2 - 0.08367E\text{-}6\ T^3 - 211708\ T^{-1} + 353.332E20\ T^{-9}$

(429.7485 < T < 3800)

BCC_A2

$-6178.89 + 91.538115\ T - 21.8386\ T\ln(T) - 5.72566E\text{-}3\ T^2 - 2.120321E\text{-}6\ T^3 - 22906\ T^{-1}$

(298.15 < T < 429.7485)

$-6233.514 + 123.676588\ T - 27.4562\ T\ln(T) + 0.54607E\text{-}3\ T^2 - 0.08367E\text{-}6\ T^3 - 211708\ T^{-1} + 353.332E20\ T^{-9}$

(429.7485 < T < 3800)

FCC_A1

$-6816.829 + 92.338115\ T - 21.8386\ T\ln(T) - 5.72566E\text{-}3\ T^2 - 2.120321E\text{-}6\ T^3 - 22906\ T^{-1}$

(298.15 < T < 429.7485)

$-6871.453 + 124.476588\ T - 27.4562\ T\ln(T) + 0.54607E\text{-}3\ T^2 - 0.08367E\text{-}6\ T^3 - 211708\ T^{-1} + 353.332E20\ T^{-9}$

(429.7485 < T < 3800)

HCP_A3

$-6445.89 + 91.651315\ T - 21.8386\ T\ln(T) - 5.72566E\text{-}3\ T^2 - 2.120321E\text{-}6\ T^3 - 22906\ T^{-1}$

(298.15 < T < 429.7485)

$-6500.514 + 123.789788\ T - 27.4562\ T\ln(T) + 0.54607E\text{-}3\ T^2 - 0.08367E\text{-}6\ T^3 - 211708\ T^{-1} + 353.332E20\ T^{-9}$

(429.7485 < T < 3800)

HCP_ZN

$-6445.89 + 91.651315\ T - 21.8386\ T\ln(T) - 5.72566E\text{-}3\ T^2 - 2.120321E\text{-}6\ T^3 - 22906\ T^{-1}$

(298.15 < T < 429.7485)

$-6500.514 + 123.789788\ T - 27.4562\ T \ln(T) + 0.54607E-3\ T^2 - 0.08367E-6\ T^3 - 211708\ T^{-1}$
$+ 353.332E20\ T^{-9}$ *(429.7485 < T < 3800)*

DHCP

$-6458.89 + 91.954115\ T - 21.8386\ T \ln(T) - 5.72566E-3\ T^2 - 2.120321E-6\ T^3 - 22906\ T^{-1}$
(298.15 < T < 429.7485)
$-6513.514 + 124.092588\ T - 27.4562\ T \ln(T) + 0.54607E-3\ T^2 - 0.08367E-6\ T^3 - 211708\ T^{-1}$
$+ 353.332E20\ T^{-9}$ *(429.7485 < T < 3800)*

Data relative to TETRAGONAL_A6

LIQUID

$3282.091 - 7.636885\ T - 559.405E-22\ T^7$ *(298.15 < T < 429.7485)*
$3283.706 - 7.640832\ T - 353.332E20\ T^{-9}$ *(429.7485 < T < 3800)*

BCT_A5

5040.87 - 3.33969 T *(298.15 < T < 3800)*

RHOMBOHEDRAL_A7

4184 *(298.15 < T < 3800)*

TET_ALPHA1

123 - 0.1988 T *(298.15 < T < 3800)*

BCC_A2

800 - 0.8 T *(298.15 < T < 3800)*

FCC_A1

162.061 *(298.15 < T < 3800)*

HCP_A3

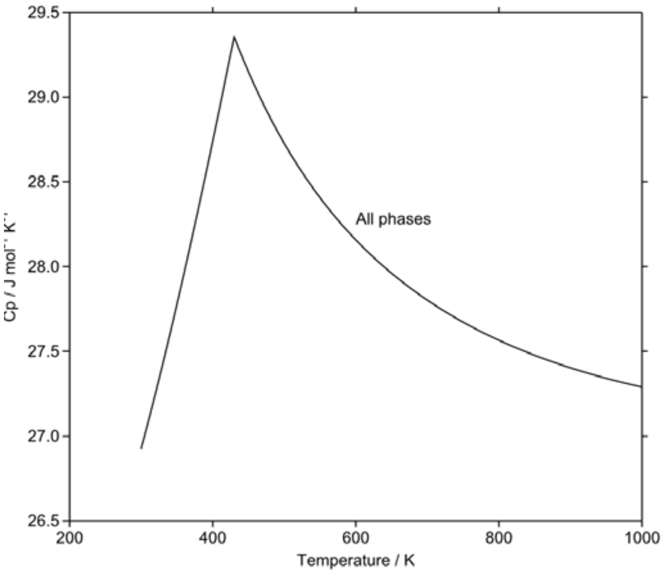
533 - 0.6868 T *(298.15 < T < 3800)*

HCP_ZN

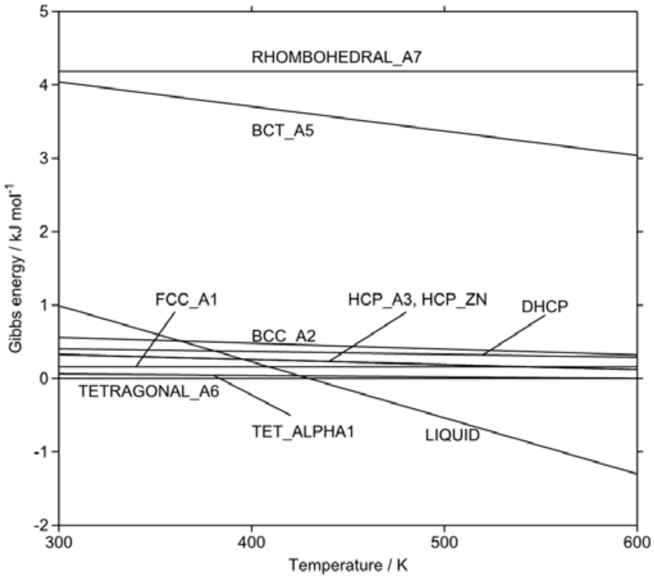
533 - 0.6868 T *(298.15 < T < 3800)*

DHCP

$520 - 0.384\ T$ *(298.15 < T < 3800)*



Heat capacity of In



Gibbs energy of phases of In relative to TETRAGONAL_A6

Ir

Source of data: *A T Dinsdale, Unpublished work [FCC_A1, LIQUID]*
Saunders et al. [BCC_A2, HCP_A3]

LIQUID

$16518.956 + 112.46806\ T - 22.7944\ T\ln(T) - 3.091976E\text{-}3\ T^2 - 20083\ T^{-1}$ *(298.15 < T < 1000)*
$102217.789 - 587.632815\ T + 73.9517579\ T\ln(T) - 46.38802E\text{-}3\ T^2 + 2.761831E\text{-}6\ T^3 - 13382612\ T^{-1}$
(1000 < T < 2719)
$-38347.217 + 411.234043\ T - 59.418\ T\ln(T)$ *(2719 < T < 4000)*

BCC_A2

$25063.712 + 111.880119\ T - 22.7944\ T\ln(T) - 3.091976E\text{-}3\ T^2 - 20083\ T^{-1}$ *(298.15 < T < 1215)*
$23876.27 + 133.166697\ T - 26.085\ T\ln(T) - 0.47969E\text{-}6\ T^3$ *(1215 < T < 2719)*
$322529.037 - 1265.252965\ T + 152.4988737\ T\ln(T) - 47.176402E\text{-}3\ T^2 + 1.844977E\text{-}6\ T^3$
$- 92987250\ T^{-1}$ *(2719 < T < 4000)*

FCC_A1

$-6936.288 + 118.780119\ T - 22.7944\ T\ln(T) - 3.091976E\text{-}3\ T^2 - 20083\ T^{-1}$ *(298.15 < T < 1215)*
$-8123.73 + 140.066697\ T - 26.085\ T\ln(T) - 0.47969E\text{-}6\ T^3$ *(1215 < T < 2719)*
$290529.037 - 1258.352965\ T + 152.4988737\ T\ln(T) - 47.176402E\text{-}3\ T^2 + 1.844977E\text{-}6\ T^3$
$- 92987250\ T^{-1}$ *(2719 < T < 4000)*

HCP_A3

$-2936.288 + 118.180119\ T - 22.7944\ T \ln(T) - 3.091976E\text{-}3\ T^2 - 20083\ T^{-1}$ *(298.15 < T < 1215)*
$-4123.73 + 139.466697\ T - 26.085\ T \ln(T) - 0.47969E\text{-}6\ T^3$ *(1215 < T < 2719)*
$294529.037 - 1258.952965\ T + 152.4988737\ T \ln(T) - 47.176402E\text{-}3\ T^2 + 1.844977E\text{-}6\ T^3$
$- 92987250\ T^{-1}$ *(2719 < T < 4000)*

Data relative to FCC_A1

LIQUID

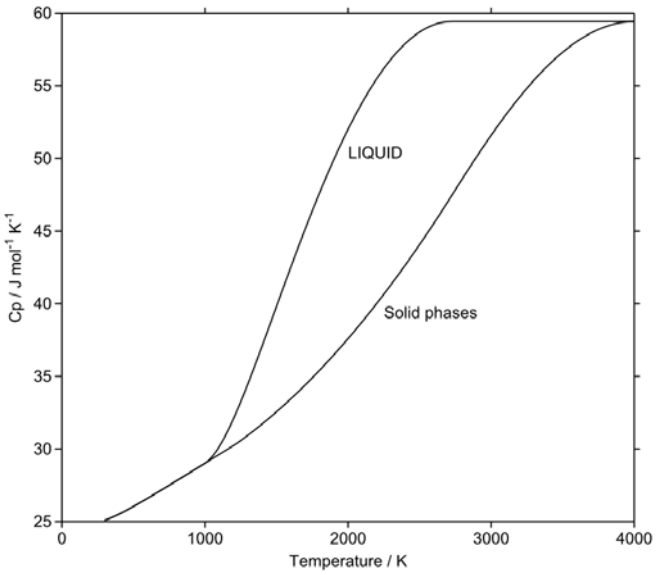
$23455.244 - 6.312059\ T$ *(298.15 < T < 1000)*
$109154.077 - 706.412934\ T + 96.7461579\ T \ln(T) - 43.296044E\text{-}3\ T^2 + 2.761831E\text{-}6\ T^3 - 13362529\ T^{-1}$
(1000 < T < 1215)
$110341.519 - 727.699512\ T + 100.0367579\ T \ln(T) - 46.38802E\text{-}3\ T^2 + 3.241521E\text{-}6\ T^3 - 13382612\ T^{-1}$
(1215 < T < 2719)
$-328876.254 + 1669.587008\ T - 211.9168737\ T \ln(T) + 47.176402E\text{-}3\ T^2 - 1.844977E\text{-}6\ T^3$
$+ 92987250\ T^{-1}$ *(2719 < T < 4000)*

BCC_A2

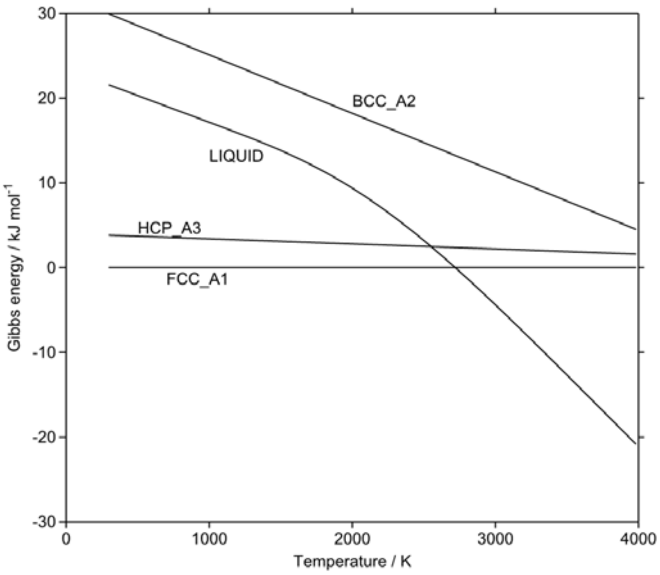
$32000 - 6.9\ T$ *(298.15 < T < 4000)*

HCP_A3

$4000 - 0.6\ T$ *(298.15 < T < 4000)*



Heat capacity of Ir



Gibbs energy of phases of Ir relative to FCC_A1

K

Source of data: *TPIS [BCC_A2, LIQUID]*
Saunders et al. [FCC_A1, HCP_A3]

BCC_A2

$-16112.929 + 389.624197\ T - 77.0571464\ T \ln(T) + 146.211135E\text{-}3\ T^2 - 84.949147E\text{-}6\ T^3 + 243385\ T^{-1}$ *(200 < T < 336.53)*

$-11122.441 + 192.586544\ T - 39.2885968\ T \ln(T) + 12.167386E\text{-}3\ T^2 - 2.64387E\text{-}6\ T^3 + 43251\ T^{-1} + 119.223E20\ T^{-9}$ *(336.53 < T < 2200)*

LIQUID

$-13794.833 + 382.737338\ T - 77.0571464\ T \ln(T) + 146.211135E\text{-}3\ T^2 - 84.949147E\text{-}6\ T^3 + 243385\ T^{-1} - 94.4E\text{-}20\ T^7$ *(200 < T < 336.53)*

$-8799.422 + 185.684327\ T - 39.2885968\ T \ln(T) + 12.167386E\text{-}3\ T^2 - 2.64387E\text{-}6\ T^3 + 43251\ T^{-1}$ *(336.53 < T < 2200)*

FCC_A1

$-16062.929 + 390.924197\ T - 77.0571464\ T \ln(T) + 146.211135E\text{-}3\ T^2 - 84.949147E\text{-}6\ T^3 + 243385\ T^{-1}$ *(200 < T < 336.53)*

$-11072.441 + 193.886544\ T - 39.2885968\ T \ln(T) + 12.167386E\text{-}3\ T^2 - 2.64387E\text{-}6\ T^3 + 43251\ T^{-1} + 119.223E20\ T^{-9}$ *(336.53 < T < 2200)*

HCP_A3

$-16062.929 + 391.624197\ T - 77.0571464\ T \ln(T) + 146.211135E\text{-}3\ T^2 - 84.949147E\text{-}6\ T^3 + 243385\ T^{-1}$ *(200 < T < 336.53)*

$-11072.441 + 194.586544\ T - 39.2885968\ T \ln(T) + 12.167386E\text{-}3\ T^2 - 2.64387E\text{-}6\ T^3 + 43251\ T^{-1} + 119.223E20\ T^{-9}$ *(336.53 < T < 2200)*

Data relative to BCC_A2

LIQUID

$2318.096 - 6.886859\ T - 94.4E\text{-}20\ T^7$ *(200 < T < 336.53)*

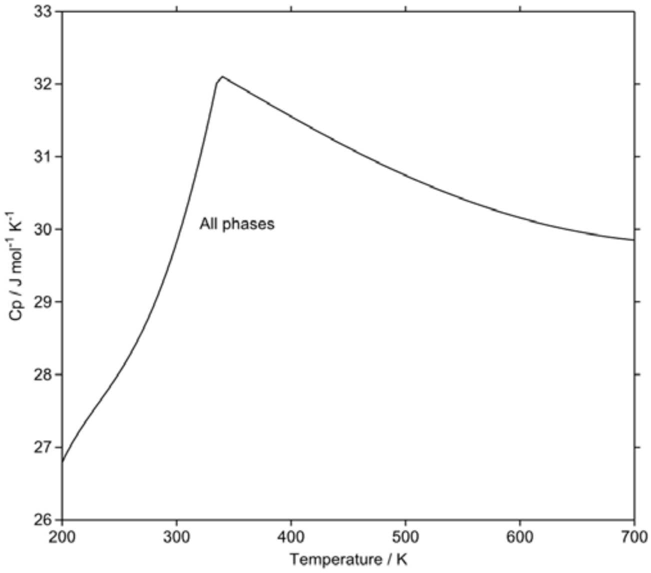
$2323.019 - 6.902217\ T - 119.223E20\ T^{-9}$ *(336.53 < T < 2200)*

FCC_A1

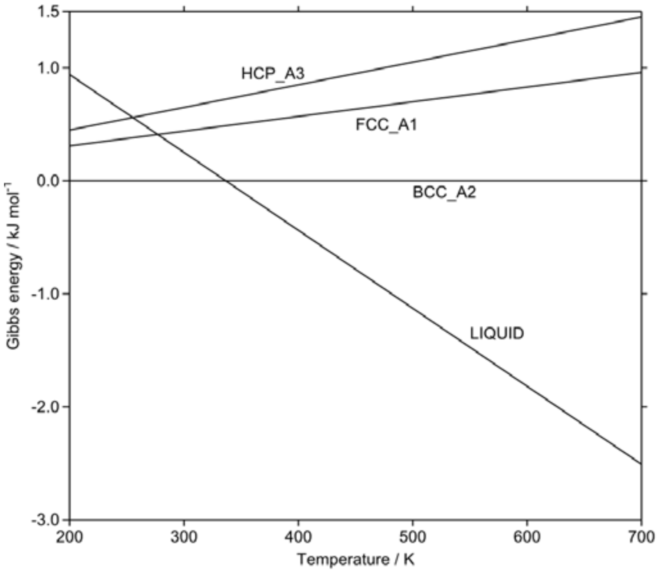
$50 + 1.3\ T$ *(200 < T < 2200)*

HCP_A3

$50 + 2\ T$ *(200 < T < 2200)*



Heat capacity of K



Gibbs energy of phases of K relative to BCC_A2

La

Source of data: *Hultgren, modified by A T Dinsdale [DHCP, FCC_A1, BCC_A2, LIQUID]*

DHCP

$-7968.403 + 120.284604\ T - 26.34\ T\ln(T) - 1.295165E-3\ T^2$ *(298.15 < T < 550)*
$-3381.413 + 59.06113\ T - 17.1659411\ T\ln(T) - 8.371705E-3\ T^2 + 0.68932E-6\ T^3 - 399448\ T^{-1}$
(550 < T < 2000)
$-15608.882 + 181.390071\ T - 34.3088\ T\ln(T)$ *(2000 < T < 4000)*

FCC_A1

$-6109.797 + 89.878761\ T - 21.7919\ T\ln(T) - 4.045175E-3\ T^2 - 0.525865E-6\ T^3$ *(298.15 < T < 1134)*
$-124598.976 + 955.878375\ T - 139.3467411\ T\ln(T) + 42.032405E-3\ T^2 - 3.066199E-6\ T^3$
$+ 20994153\ T^{-1}$ *(1134 < T < 2000)*
$-12599.386 + 178.54399\ T - 34.3088\ T\ln(T)$ *(2000 < T < 4000)*

BCC_A2

$-3952.161 + 88.072353\ T - 21.7919\ T\ln(T) - 4.045175E-3\ T^2 - 0.525865E-6\ T^3$ *(298.15 < T < 800)*
$321682.673 - 3565.082518\ T + 513.4407077\ T\ln(T) - 387.295093E-3\ T^2 + 49.547989E-6\ T^3$
$- 36581228\ T^{-1}$ *(800 < T < 1134)*
$-16377.894 + 218.492988\ T - 39.5388\ T\ln(T)$ *(1134 < T < 1193)*
$-136609.91 + 1123.343974\ T - 163.4130738\ T\ln(T) + 53.968535E-3\ T^2 - 4.056395E-6\ T^3$
$+ 21167204\ T^{-1}$ *(1193 < T < 2000)*
$-8205.988 + 174.836315\ T - 34.3088\ T\ln(T)$ *(2000 < T < 4000)*

LIQUID

$5332.653 + 18.23012\ T - 11.0188191\ T \ln(T) - 20.171603E\text{-}3\ T^2 + 2.93775E\text{-}6\ T^3 - 133541\ T^{-1}$ *(298.15 < T < 1134)*

$-3942.004 + 171.018431\ T - 34.3088\ T \ln(T)$ *(1134 < T < 4000)*

Data relative to DHCP

FCC_A1

$1858.606 - 30.405843\ T + 4.5481\ T \ln(T) - 2.75001E\text{-}3\ T^2 - 0.525865E\text{-}6\ T^3$ *(298.15 < T < 550)*

$-2728.384 + 30.817631\ T - 4.6259589\ T \ln(T) + 4.32653E\text{-}3\ T^2 - 1.215185E\text{-}6\ T^3 + 399448\ T^{-1}$ *(550 < T < 1134)*

$-121217.563 + 896.817245\ T - 122.1808\ T \ln(T) + 50.40411E\text{-}3\ T^2 - 3.755519E\text{-}6\ T^3 + 21393601\ T^{-1}$ *(1134 < T < 2000)*

$3009.496 - 2.846081\ T$ *(2000 < T < 4000)*

BCC_A2

$4016.242 - 32.212251\ T + 4.5481\ T \ln(T) - 2.75001E\text{-}3\ T^2 - 0.525865E\text{-}6\ T^3$ *(298.15 < T < 550)*

$-570.748 + 29.011223\ T - 4.6259589\ T \ln(T) + 4.32653E\text{-}3\ T^2 - 1.215185E\text{-}6\ T^3 + 399448\ T^{-1}$ *(550 < T < 800)*

$325064.086 - 3624.143648\ T + 530.6066488\ T \ln(T) - 378.923388E\text{-}3\ T^2 + 48.858669E\text{-}6\ T^3 - 36181780\ T^{-1}$ *(800 < T < 1134)*

$-12996.481 + 159.431858\ T - 22.3728589\ T \ln(T) + 8.371705E\text{-}3\ T^2 - 0.68932E\text{-}6\ T^3 + 399448\ T^{-1}$ *(1134 < T < 1193)*

$-133228.497 + 1064.282844\ T - 146.2471327\ T \ln(T) + 62.34024E\text{-}3\ T^2 - 4.745715E\text{-}6\ T^3 + 21566652\ T^{-1}$ *(1193 < T < 2000)*

$7402.894 - 6.553756\ T$ *(2000 < T < 4000)*

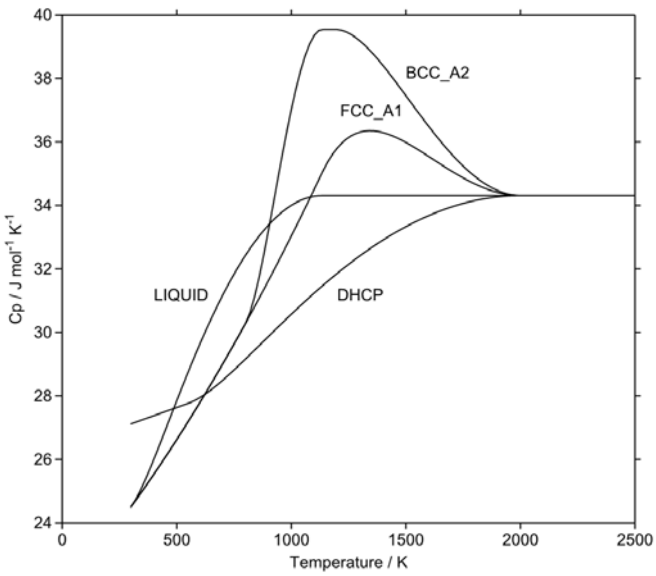
LIQUID

$13301.056 - 102.054484\ T + 15.3211809\ T \ln(T) - 18.876438E\text{-}3\ T^2 + 2.93775E\text{-}6\ T^3 - 133541\ T^{-1}$ *(298.15 < T < 550)*

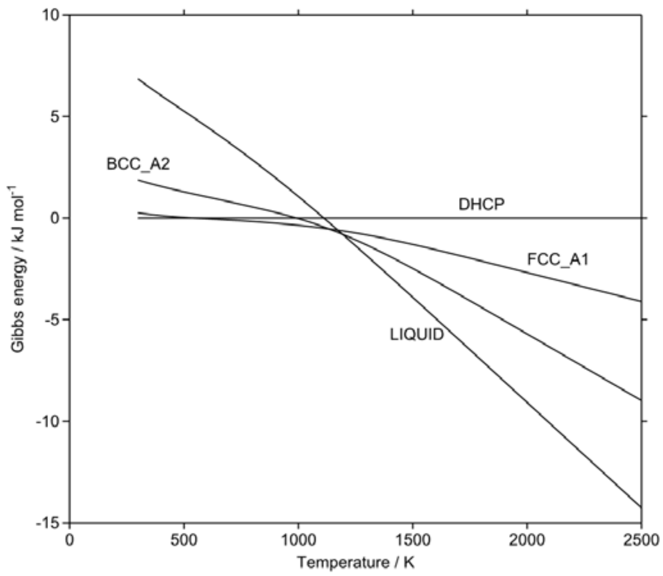
$8714.066 - 40.83101\ T + 6.147122\ T \ln(T) - 11.799898E\text{-}3\ T^2 + 2.24843E\text{-}6\ T^3 + 265907\ T^{-1}$ *(550 < T < 1134)*

$-560.591 + 111.957301\ T - 17.1428589\ T \ln(T) + 8.371705E\text{-}3\ T^2 - 0.68932E\text{-}6\ T^3 + 399448\ T^{-1}$ *(1134 < T < 2000)*

$11666.878 - 10.37164\ T$ *(2000 < T < 4000)*



Heat capacity of La



Gibbs energy of phases of La relative to DHCP

Li

Source of data: *TPIS [BCC_A2, LIQUID]*
Saunders et al. [FCC_A1, HCP_A3]

BCC_A2

-10583.817 + 217.637482 T - 38.940488 T ln(T) + 35.466931E-3 T^2 - 19.869816E-6 T^3 + 159994 T^{-1}
(200 < T < 453.6)
-559579.123 + 10547.879893 T - 1702.8886493 T ln(T) + 2258.329444E-3 T^2 - 571.066077E-6 T^3
+ 33885874 T^{-1} *(453.6 < T < 500)*
-9062.994 + 179.278285 T - 31.2283718 T ln(T) + 2.633221E-3 T^2 - 0.438058E-6 T^3 - 102387 T^{-1}
(500 < T < 3000)

LIQUID

-7883.612 + 211.841861 T - 38.940488 T ln(T) + 35.466931E-3 T^2 - 19.869816E-6 T^3 + 159994 T^{-1}
(200 < T < 250)
12015.027 - 362.187078 T + 61.6104424 T ln(T) - 182.426463E-3 T^2 + 63.955671E-6 T^3 - 559968 T^{-1}
(250 < T < 453.6)
-6057.31 + 172.652183 T - 31.2283718 T ln(T) + 2.633221E-3 T^2 - 0.438058E-6 T^3 - 102387 T^{-1}
(453.6 < T < 3000)

FCC_A1

-10691.817 + 218.937482 T - 38.940488 T ln(T) + 35.466931E-3 T^2 - 19.869816E-6 T^3 + 159994 T^{-1}
(200 < T < 453.6)
-559687.123 + 10549.179893 T - 1702.8886493 T ln(T) + 2258.329444E-3 T^2 - 571.066077E-6 T^3
+ 33885874 T^{-1} *(453.6 < T < 500)*

$-9170.994 + 180.578285\ T - 31.2283718\ T \ln(T) + 2.633221E\text{-}3\ T^2 - 0.438058E\text{-}6\ T^3 - 102387\ T^{-1}$
(500 < T < 3000)

HCP_A3

$-10737.817 + 219.637482\ T - 38.940488\ T \ln(T) + 35.466931E\text{-}3\ T^2 - 19.869816E\text{-}6\ T^3 + 159994\ T^{-1}$
(200 < T < 453.6)
$-559733.123 + 10549.879893\ T - 1702.8886493\ T \ln(T) + 2258.329444E\text{-}3\ T^2 - 571.066077E\text{-}6\ T^3$
$+ 33885874\ T^{-1}$ *(453.6 < T < 500)*
$-9216.994 + 181.278285\ T - 31.2283718\ T \ln(T) + 2.633221E\text{-}3\ T^2 - 0.438058E\text{-}6\ T^3 - 102387\ T^{-1}$
(500 < T < 3000)

Data relative to BCC_A2

LIQUID

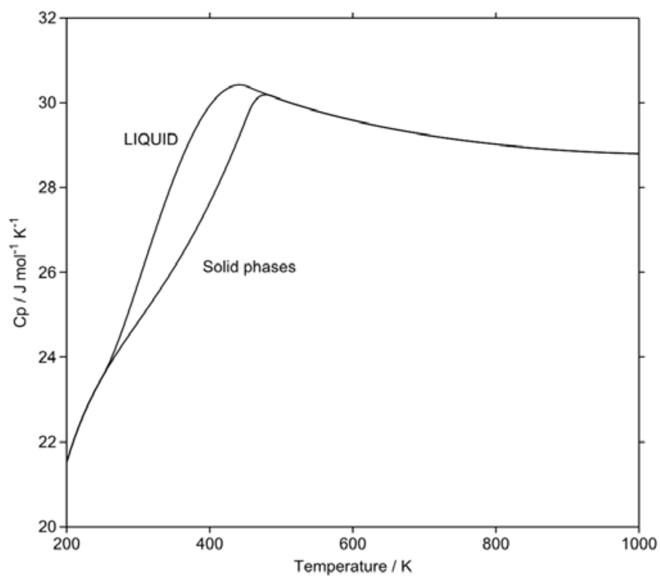
$2700.205 - 5.795621\ T$ *(200 < T < 250)*
$22598.844 - 579.82456\ T + 100.5509304\ T \ln(T) - 217.893394E\text{-}3\ T^2 + 83.825487E\text{-}6\ T^3 - 719962\ T^{-1}$
(250 < T < 453.6)
$553521.813 - 10375.22771\ T + 1671.6602775\ T \ln(T) - 2255.696223E\text{-}3\ T^2 + 570.628019E\text{-}6\ T^3$
$- 33988261\ T^{-1}$ *(453.6 < T < 500)*
$3005.684 - 6.626102\ T$ *(500 < T < 3000)*

FCC_A1

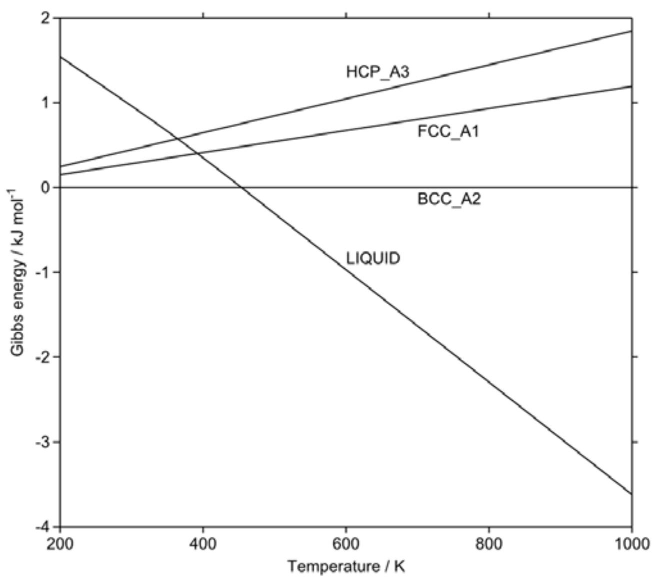
$-108 + 1.3\ T$ *(200 < T < 3000)*

HCP_A3

$-154 + 2\ T$ *(200 < T < 3000)*



Heat capacity of Li



Gibbs energy of phases of Li relative to BCC_A2

Lu

Source of data: *Hultgren [HCP_A3, LIQUID]*

HCP_A3

$-8788.329 + 146.536283\ T - 29.812\ T\ \ln(T) + 5.19165E\text{-}3\ T^2 - 1.790717E\text{-}6\ T^3 + 39723\ T^{-1}$ *(298.15 < T < 700)*

$-9043.057 + 142.327643\ T - 29.0095\ T\ \ln(T) + 3.71416E\text{-}3\ T^2 - 1.50147E\text{-}6\ T^3 + 141549\ T^{-1}$ *(700 < T < 1700)*

$6940.092 - 46.91844\ T - 1.83986\ T\ \ln(T) - 11.9001E\text{-}3\ T^2$ *(1700 < T < 1936)*

$-404023.691 + 1829.379425\ T - 239.019502\ T\ \ln(T) + 41.800748E\text{-}3\ T^2 - 1.661174E\text{-}6\ T^3 + 124825465\ T^{-1}$ *(1936 < T < 3700)*

LIQUID

$3983.791 + 141.5374\ T - 29.812\ T\ \ln(T) + 5.19165E\text{-}3\ T^2 - 1.790717E\text{-}6\ T^3 + 39723\ T^{-1}$ *(298.15 < T < 600)*

$30389.863 - 198.378793\ T + 20.9392663\ T\ \ln(T) - 34.238743E\text{-}3\ T^2 + 2.890636E\text{-}6\ T^3 - 2398650\ T^{-1}$ *(600 < T < 1936)*

$-18994.687 + 292.091104\ T - 47.9068\ T\ \ln(T)$ *(1936 < T < 3700)*

Data relative to HCP_A3

LIQUID

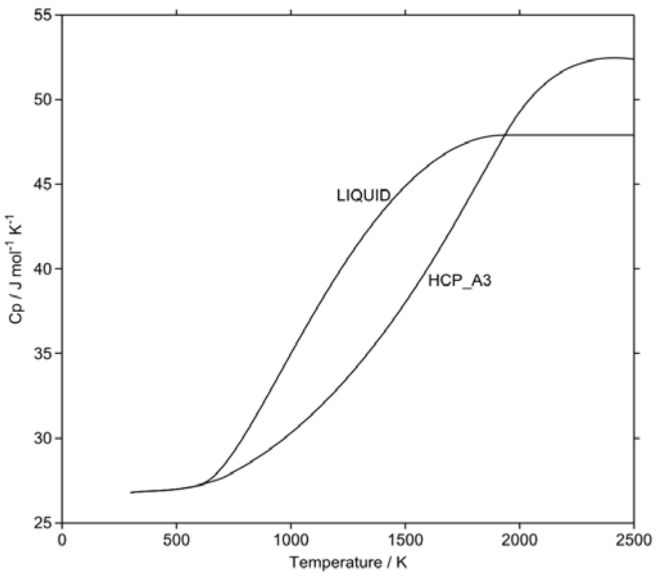
$12772.12 - 4.998883\ T$ *(298.15 < T < 600)*

$39178.192 - 344.915076\ T + 50.7512663\ T\ \ln(T) - 39.430393E\text{-}3\ T^2 + 4.681353E\text{-}6\ T^3 - 2438373\ T^{-1}$ *(600 < T < 700)*

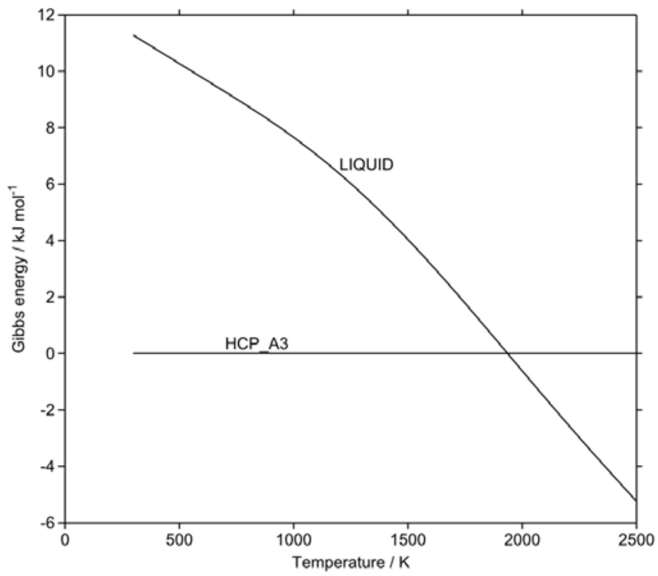
$39432.92 - 340.706436\ T + 49.9487663\ T\ \ln(T) - 37.952903E\text{-}3\ T^2 + 4.392106E\text{-}6\ T^3 - 2540199\ T^{-1}$ *(700 < T < 1700)*

$23449.771 - 151.460353\ T + 22.7791263\ T\ \ln(T) - 22.338643E\text{-}3\ T^2 + 2.890636E\text{-}6\ T^3 - 2398650\ T^{-1}$ *(1700 < T < 1936)*

$385029.004 - 1537.288321\ T + 191.112702\ T\ \ln(T) - 41.800748E\text{-}3\ T^2 + 1.661174E\text{-}6\ T^3 - 124825465\ T^{-1}$ *(1936 < T < 3700)*



Heat capacity of Lu



Gibbs energy of phases of Lu relative to HCP_A3

Mg

Source of data: *CODATA [HCP_A3, LIQUID]*
Hack (unpublished work) [BCC_A12]
Tibbals (unpublished work) [CUB_A13]
Saunders et al. [BCC_A2, FCC_A1]

HCP_A3

$-8367.34 + 143.675547\ T - 26.1849782\ T\ln(T) + 0.4858E{-3}\ T^2 - 1.393669E{-6}\ T^3 + 78950\ T^{-1}$ *(298.15 < T < 923)*

$-14130.185 + 204.716215\ T - 34.3088\ T\ln(T) + 1038.192E25\ T^{-9}$ *(923 < T < 3000)*

LIQUID

$-165.097 + 134.838617\ T - 26.1849782\ T\ln(T) + 0.4858E{-3}\ T^2 - 1.393669E{-6}\ T^3 + 78950\ T^{-1} - 80.176E{-21}\ T^7$ *(298.15 < T < 923)*

$-5439.869 + 195.324057\ T - 34.3088\ T\ln(T)$ *(923 < T < 3000)*

BCC_A2

$-5267.34 + 141.575547\ T - 26.1849782\ T\ln(T) + 0.4858E{-3}\ T^2 - 1.393669E{-6}\ T^3 + 78950\ T^{-1}$ *(298.15 < T < 923)*

$-11030.185 + 202.616215\ T - 34.3088\ T\ln(T) + 1038.192E25\ T^{-9}$ *(923 < T < 3000)*

CBCC_A12

$-3764.94 + 140.664547\ T - 26.1849782\ T\ln(T) + 0.4858E{-3}\ T^2 - 1.393669E{-6}\ T^3 + 78950\ T^{-1}$ *(298.15 < T < 923)*

$-9527.785 + 201.705215\ T - 34.3088\ T\ \ln(T) + 1038.192E25\ T^{-9}$ *(923 < T < 3000)*

CUB_A13

$-3367.34 + 140.675547\ T - 26.1849782\ T\ \ln(T) + 0.4858E-3\ T^2 - 1.393669E-6\ T^3 + 78950\ T^{-1}$ *(298.15 < T < 923)*

$-9130.185 + 201.716215\ T - 34.3088\ T\ \ln(T) + 1038.192E25\ T^{-9}$ *(923 < T < 3000)*

FCC_A1

$-5767.34 + 142.775547\ T - 26.1849782\ T\ \ln(T) + 0.4858E-3\ T^2 - 1.393669E-6\ T^3 + 78950\ T^{-1}$ *(298.15 < T < 923)*

$-11530.185 + 203.816215\ T - 34.3088\ T\ \ln(T) + 1038.192E25\ T^{-9}$ *(923 < T < 3000)*

HCP_ZN

$-8267.34 + 143.675547\ T - 26.1849782\ T\ \ln(T) + 0.4858E-3\ T^2 - 1.393669E-6\ T^3 + 78950\ T^{-1}$ *(298.15 < T < 923)*

$-14030.185 + 204.716215\ T - 34.3088\ T\ \ln(T) + 1038.192E25\ T^{-9}$ *(923 < T < 3000)*

Data relative to HCP_A3

LIQUID

$8202.243 - 8.83693\ T - 80.176E-21\ T^7$ *(298.15 < T < 923)*

$8690.316 - 9.392158\ T - 1038.192E25\ T^{-9}$ *(923 < T < 3000)*

BCC_A2

$3100 - 2.1\ T$ *(298.15 < T < 3000)*

CBCC_A12

$4602.4 - 3.011\ T$ *(298.15 < T < 3000)*

CUB_A13

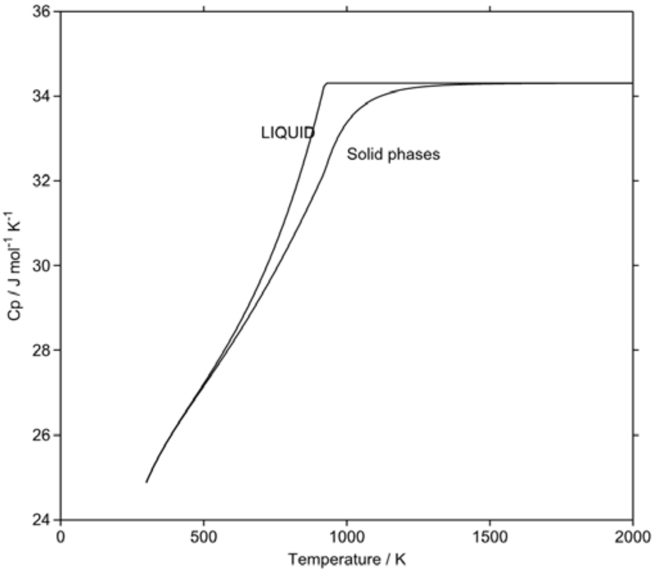
$5000 - 3\ T$ *(298.15 < T < 3000)*

FCC_A1

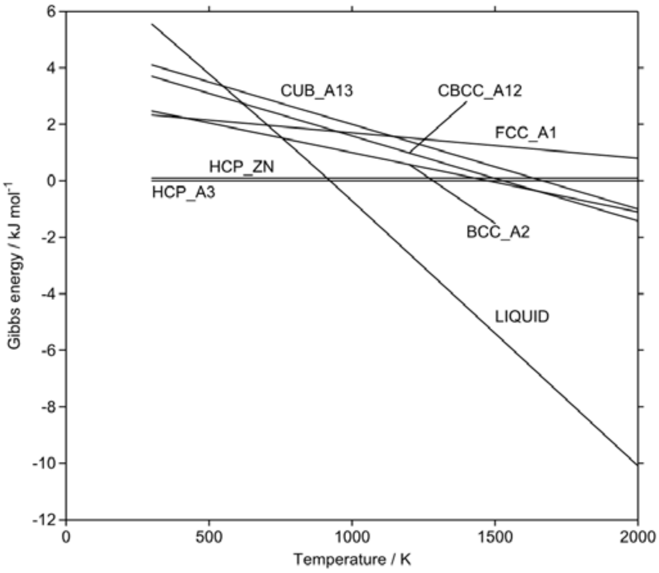
$2600 - 0.9\ T$ *(298.15 < T < 3000)*

HCP_ZN

100 *(298.15 < T < 3000)*



Heat capacity of Mg



Gibbs energy of phases of Mg relative to HCP_A3

Mn

Source of data: *A Fernandez Guillermet, W Huang, Int. J. Thermophys., 1990,* ***11****, 949-69 [BCC_A12, CUB_A13, FCC_A1, BCC_A2, LIQUID]*
Saunders et al. [HCP_A3]

CBCC_A12

$T_N = 95$ $B_0 = 0.22$

$-8115.28 + 130.059\ T - 23.4582\ T \ln(T) - 7.34768E\text{-}3\ T^2 + 69827\ T^{-1} + Gmag$ *(298.15 < T < 1519)*
$-28733.41 + 312.2648\ T - 48\ T \ln(T) + 1656.847E27\ T^{-9} + Gmag$ *(1519 < T < 2000)*

CUB_A13

$-5800.4 + 135.995\ T - 24.8785\ T \ln(T) - 5.83359E\text{-}3\ T^2 + 70269\ T^{-1}$ *(298.15 < T < 1519)*
$-28290.76 + 311.2933\ T - 48\ T \ln(T) + 396.757E28\ T^{-9}$ *(1519 < T < 2000)*

FCC_A1

$T_N = 540$ $B_0 = 0.62$

$-3439.3 + 131.884\ T - 24.5177\ T \ln(T) - 6E\text{-}3\ T^2 + 69600\ T^{-1} + Gmag$ *(298.15 < T < 1519)*
$-26070.1 + 309.6664\ T - 48\ T \ln(T) + 386.196E28\ T^{-9} + Gmag$ *(1519 < T < 2000)*

BCC_A2

$T_N = 580$ $B_0 = 0.27$

$-3235.3 + 127.85\ T - 23.7\ T \ln(T) - 7.44271E\text{-}3\ T^2 + 60000\ T^{-1} + Gmag$ *(298.15 < T < 1519)*

$-23188.83 + 307.7043\ T - 48\ T \ln(T) + 1265.152E27\ T^{-9} + Gmag$ *(1519 < T < 2000)*

LIQUID

$9744.63 + 117.4382\ T - 23.4582\ T \ln(T) - 7.34768E\text{-}3\ T^{2} + 69827\ T^{-1} - 441.929E\text{-}23\ T^{7}$
(298.15 < T < 1519)
$-9993.9 + 299.036\ T - 48\ T \ln(T)$ *(1519 < T < 2000)*

HCP_A3

$T_N = 540$ $B_0 = 0.62$

$-4439.3 + 133.007\ T - 24.5177\ T \ln(T) - 6E\text{-}3\ T^{2} + 69600\ T^{-1} + Gmag$ *(298.15 < T < 1519)*
$-27070.1 + 310.7894\ T - 48\ T \ln(T) + 386.196E28\ T^{-9} + Gmag$ *(1519 < T < 2000)*

Data relative to paramagnetic CBCC_A12

CBCC_A12

$T_N = 95$ $B_0 = 0.22$

Gmag *(298.15 < T < 2000)*

CUB_A13

$2314.88 + 5.936\ T - 1.4203\ T \ln(T) + 1.51409E\text{-}3\ T^{2} + 442\ T^{-1}$ *(298.15 < T < 1519)*
$442.65 - 0.9715\ T + 2310.723E27\ T^{-9}$ *(1519 < T < 2000)*

FCC_A1

$T_N = 540$ $B_0 = 0.62$

$4675.98 + 1.825\ T - 1.0595\ T \ln(T) + 1.34768E\text{-}3\ T^{2} - 227\ T^{-1} + Gmag$ *(298.15 < T < 1519)*
$2663.31 - 2.5984\ T + 2205.113E27\ T^{-9} + Gmag$ *(1519 < T < 2000)*

BCC_A2

$T_N = 580$ $B_0 = 0.27$

$4879.98 - 2.209\ T - 0.2418\ T \ln(T) - 0.09503E\text{-}3\ T^{2} - 9827\ T^{-1} + Gmag$ *(298.15 < T < 1519)*
$5544.58 - 4.5605\ T - 391.695E27\ T^{-9} + Gmag$ *(1519 < T < 2000)*

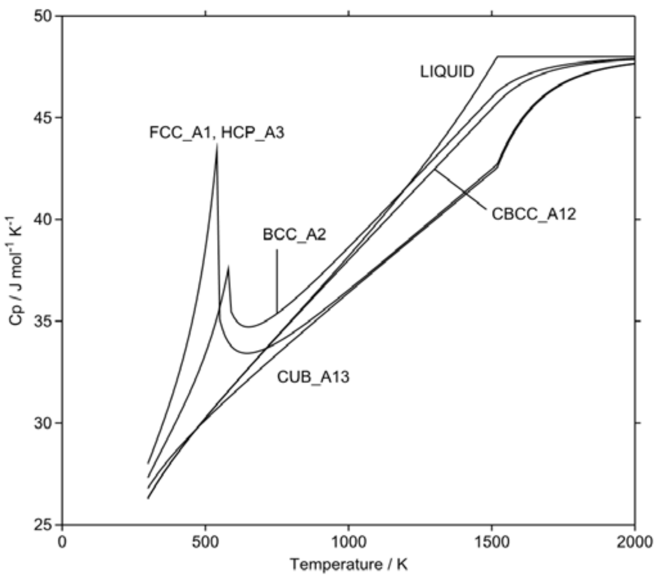
LIQUID

$17859.91 - 12.6208\ T - 441.929E\text{-}23\ T^{7}$ *(298.15 < T < 1519)*
$18739.51 - 13.2288\ T - 1656.847E27\ T^{-9}$ *(1519 < T < 2000)*

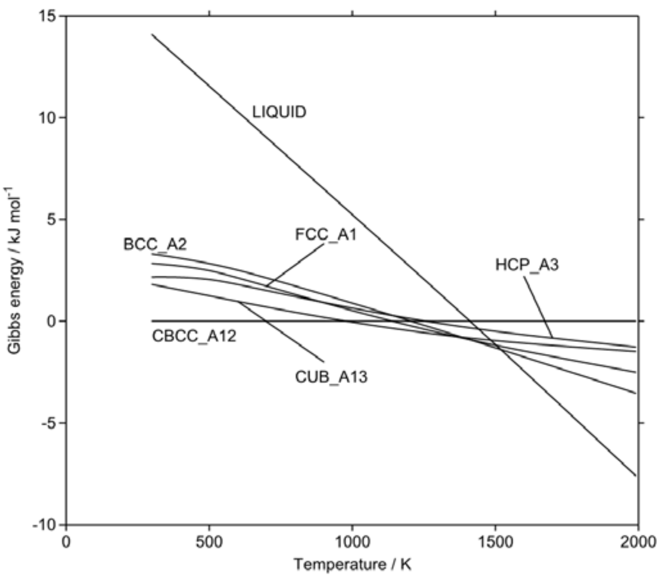
HCP_A3

$T_N = 540$ $\quad\quad$ $B_0 = 0.62$

$3675.98 + 2.948\ T - 1.0595\ T\ \ln(T) + 1.34768E\text{-}3\ T^2 - 227\ T^{-1} + Gmag$ *(298.15 < T < 1519)*
$1663.31 - 1.4754\ T + 2205.113E27\ T^{-9} + Gmag$ *(1519 < T < 2000)*



Heat capacity of Mn



Gibbs energy of phases of Mn relative to CBCC_A12

Mo

Source of data: *A Fernandez Guillermet, Int. J. Thermophys, 1985, **6**, 263-393 [BCC_A2, LIQUID]*
*J-O Andersson, A Fernandez Guillermet, P Gustafson, CALPHAD, 1987, **11**, 361-4 [HCP_A3, FCC_A1]*

BCC_A2

$A = 9.34372E\text{-}6$	$a_0 = 1.4378E\text{-}5$	$a_1 = 4.66062E\text{-}10$	$a_2 = 3.44061E\text{-}12$
$K_0 = 3.5027E\text{-}12$	$K_1 = 1.5E\text{-}16$	$K_2 = 3.9E\text{-}20$	$n = 3.25$

$-7746.302 + 131.9197\ T - 23.56414\ T\ \ln(T) - 3.443396E\text{-}3\ T^2 + 0.566283E\text{-}6\ T^3 + 65812\ T^{-1}$
$- 0.130927E\text{-}9\ T^4 + Gpres$ *(298.15 < T < 2896)*
$-30556.41 + 283.559746\ T - 42.63829\ T\ \ln(T) - 4849.315E30\ T^{-9} + Gpres$ *(2896 < T < 5000)*

LIQUID

$A = 9.75079E\text{-}6$	$a_0 = 1.4378E\text{-}5$	$a_1 = 4.66062E\text{-}10$	$a_2 = 3.44061E\text{-}12$
$K_0 = 3.5027E\text{-}12$	$K_1 = 1.5E\text{-}16$	$K_2 = 3.9E\text{-}20$	$n = 3.25$

$34085.045 + 117.224788\ T - 23.56414\ T\ \ln(T) - 3.443396E\text{-}3\ T^2 + 0.566283E\text{-}6\ T^3 + 65812\ T^{-1}$
$- 0.130927E\text{-}9\ T^4 + 424.519E\text{-}24\ T^7 + Gpres$ *(298.15 < T < 2896)*

$3538.963 + 271.6697\ T - 42.63829\ T \ln(T) + Gpres$ *(2896 < T < 5000)*

FCC_A1

$A = 9.34372E-6$	$a_0 = 1.4378E-5$	$a_1 = 4.66062E-10$	$a_2 = 3.44061E-12$
$K_0 = 3.5027E-12$	$K_1 = 1.5E-16$	$K_2 = 3.9E-20$	$n = 3.25$

$7453.698 + 132.5497\ T - 23.56414\ T \ln(T) - 3.443396E-3\ T^2 + 0.566283E-6\ T^3 + 65812\ T^{-1}$
$- 0.130927E-9\ T^4 + Gpres$ *(298.15 < T < 2896)*
$-15356.41 + 284.189746\ T - 42.63829\ T \ln(T) - 4849.315E30\ T^{-9} + Gpres$ *(2896 < T < 5000)*

HCP_A3

$A = 9.34372E-6$	$a_0 = 1.4378E-5$	$a_1 = 4.66062E-10$	$a_2 = 3.44061E-12$
$K_0 = 3.5027E-12$	$K_1 = 1.5E-16$	$K_2 = 3.9E-20$	$n = 3.25$

$3803.698 + 131.9197\ T - 23.56414\ T \ln(T) - 3.443396E-3\ T^2 + 0.566283E-6\ T^3 + 65812\ T^{-1}$
$- 0.130927E-9\ T^4 + Gpres$ *(298.15 < T < 2896)*
$-19006.41 + 283.559746\ T - 42.63829\ T \ln(T) - 4849.315E30\ T^{-9} + Gpres$ *(2896 < T < 5000)*

Data relative to BCC_A2

BCC_A2

$A = 9.34372E-6$	$a_0 = 1.4378E-5$	$a_1 = 4.66062E-10$	$a_2 = 3.44061E-12$
$K_0 = 3.5027E-12$	$K_1 = 1.5E-16$	$K_2 = 3.9E-20$	$n = 3.25$

Gpres *(298.15 < T < 5000)*

LIQUID

$A = 9.75079E-6$	$a_0 = 1.4378E-5$	$a_1 = 4.66062E-10$	$a_2 = 3.44061E-12$
$K_0 = 3.5027E-12$	$K_1 = 1.5E-16$	$K_2 = 3.9E-20$	$n = 3.25$

$41831.347 - 14.694912\ T + 424.519E-24\ T^7 + Gpres$ *(298.15 < T < 2896)*
$34095.373 - 11.890046\ T + 4849.315E30\ T^{-9} + Gpres$ *(2896 < T < 5000)*

FCC_A1

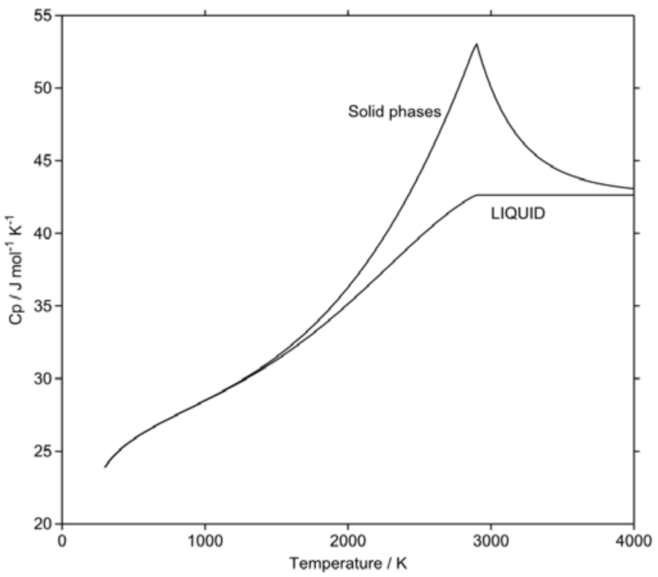
$A = 9.34372E-6$	$a_0 = 1.4378E-5$	$a_1 = 4.66062E-10$	$a_2 = 3.44061E-12$
$K_0 = 3.5027E-12$	$K_1 = 1.5E-16$	$K_2 = 3.9E-20$	$n = 3.25$

$15200 + 0.63\ T + Gpres$ *(298.15 < T < 5000)*

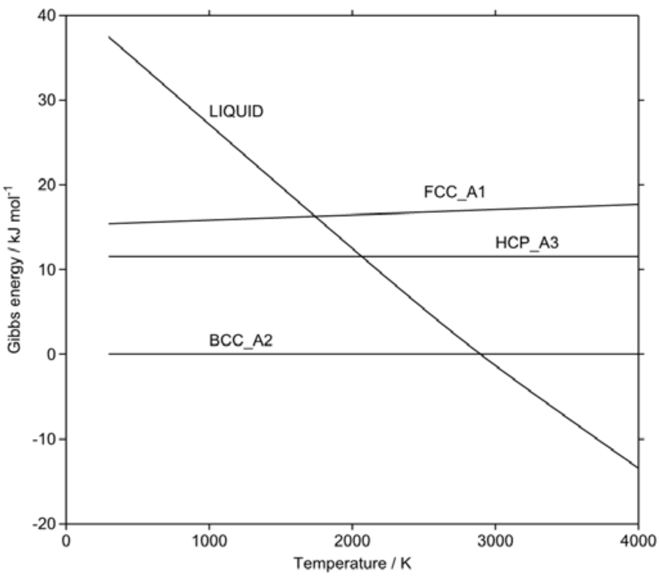
HCP_A3

$A = 9.34372E-6$	$a_0 = 1.4378E-5$	$a_1 = 4.66062E-10$	$a_2 = 3.44061E-12$
$K_0 = 3.5027E-12$	$K_1 = 1.5E-16$	$K_2 = 3.9E-20$	$n = 3.25$

$11550 + Gpres$ *(298.15 < T < 5000)*



Heat capacity of Mo



Gibbs energy of phases of Mo relative to BCC_A2

N

Source of data: *K Frisk, TRITA-MAC-0393, April 1989 [GAS, LIQUID]*

GAS (1/2N2)

-3750.675 - 9.45425 T - 12.7819 T ln(T) - 1.76686E-3 T^2 + 0.002681E-6 T^3 - 32374 T^{-1} *(298.15 < T < 950)*

-7358.85 + 17.2003 T - 16.3699 T ln(T) - 0.65107E-3 T^2 + 0.030097E-6 T^3 + 563070 T^{-1} *(950 < T < 3350)*

-16392.8 + 50.26 T - 20.4695 T ln(T) + 0.239754E-3 T^2 - 0.008333E-6 T^3 + 4596375 T^{-1} *(3350 < T < 6000)*

LIQUID

26199.325 + 49.56575 T - 12.7819 T ln(T) - 1.76686E-3 T^2 + 0.002681E-6 T^3 - 32374 T^{-1} *(298.15 < T < 950)*

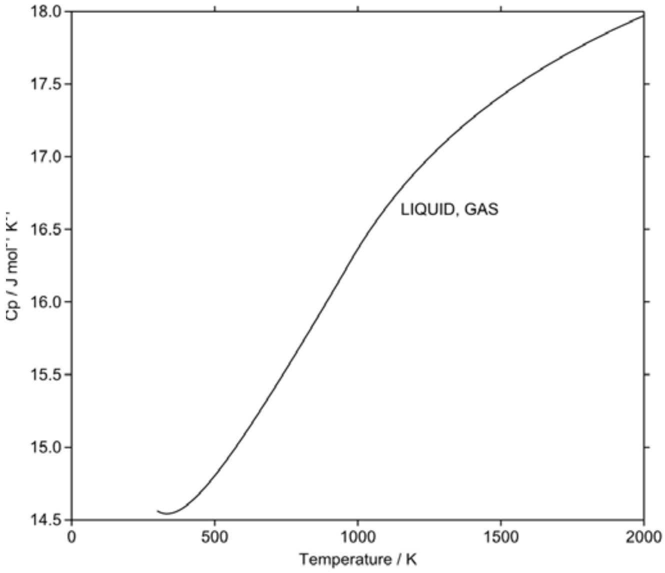
22591.15 + 76.2203 T - 16.3699 T ln(T) - 0.65107E-3 T^2 + 0.030097E-6 T^3 + 563070 T^{-1} *(950 < T < 3350)*

13557.2 + 109.28 T - 20.4695 T ln(T) + 0.239754E-3 T^2 - 0.008333E-6 T^3 + 4596375 T^{-1} *(3350 < T < 6000)*

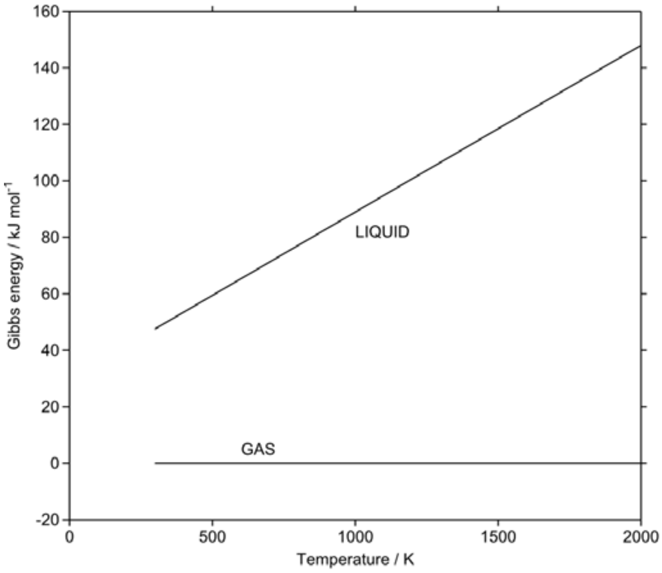
Data relative to GAS

LIQUID

29950 + 59.02 T *(298.15 < T < 6000)*



Heat capacity of N



Gibbs energy of phases of N relative to GAS

Na

Source of data: *TPIS [BCC_A2, LIQUID]*
Saunders et al. [HCP_A3, FCC_A1]

BCC_A2

$-11989.434 + 260.548732\ T - 51.0393608\ T\ln(T) + 72.306633E\text{-}3\ T^2 - 43.638283E\text{-}6\ T^3 + 132154\ T^{-1}$ *(200 < T < 370.87)*

$-11009.884 + 199.619999\ T - 38.1198801\ T\ln(T) + 9.745854E\text{-}3\ T^2 - 1.70664E\text{-}6\ T^3 + 34342\ T^{-1} + 165.071E21\ T^{-9}$ *(370.87 < T < 2300)*

LIQUID

$-9408.414 + 253.596552\ T - 51.0393608\ T\ln(T) + 72.306633E\text{-}3\ T^2 - 43.638283E\text{-}6\ T^3 + 132154\ T^{-1} - 276.132E\text{-}20\ T^7$ *(200 < T < 370.87)*

$-8400.44 + 192.587343\ T - 38.1198801\ T\ln(T) + 9.745854E\text{-}3\ T^2 - 1.70664E\text{-}6\ T^3 + 34342\ T^{-1}$ *(370.87 < T < 2300)*

FCC_A1

$-12039.434 + 261.848732\ T - 51.0393608\ T\ln(T) + 72.306633E\text{-}3\ T^2 - 43.638283E\text{-}6\ T^3 + 132154\ T^{-1}$ *(200 < T < 370.87)*

$-11059.884 + 200.919999\ T - 38.1198801\ T\ln(T) + 9.745854E\text{-}3\ T^2 - 1.70664E\text{-}6\ T^3 + 34342\ T^{-1} + 165.071E21\ T^{-9}$ *(370.87 < T < 2300)*

HCP_A3

$-12093.434 + 262.548732\ T - 51.0393608\ T\ \ln(T) + 72.306633E\text{-}3\ T^2 - 43.638283E\text{-}6\ T^3 + 132154\ T^{-1}$ *(200 < T < 370.87)*

$-11113.884 + 201.619999\ T - 38.1198801\ T\ \ln(T) + 9.745854E\text{-}3\ T^2 - 1.70664E\text{-}6\ T^3 + 34342\ T^{-1} + 165.071E21\ T^{-9}$ *(370.87 < T < 2300)*

Data relative to BCC_A2

LIQUID

$2581.02 - 6.95218\ T - 276.132E\text{-}20\ T^7$ *(200 < T < 370.87)*

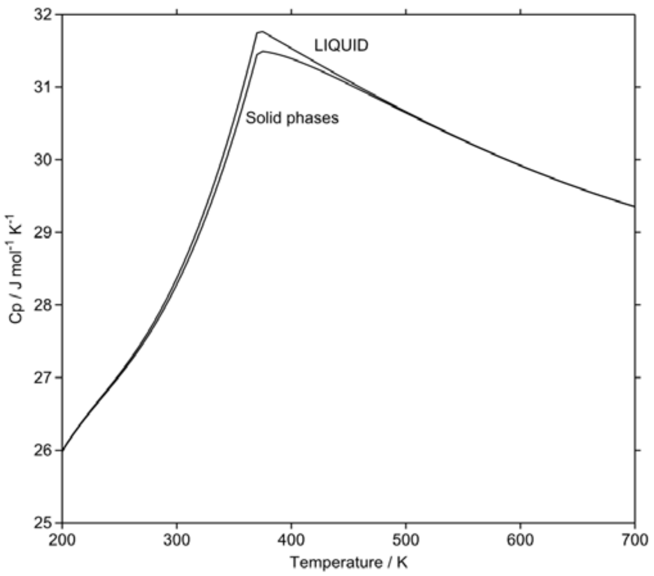
$2609.444 - 7.032656\ T - 165.071E21\ T^{-9}$ *(370.87 < T < 2300)*

FCC_A1

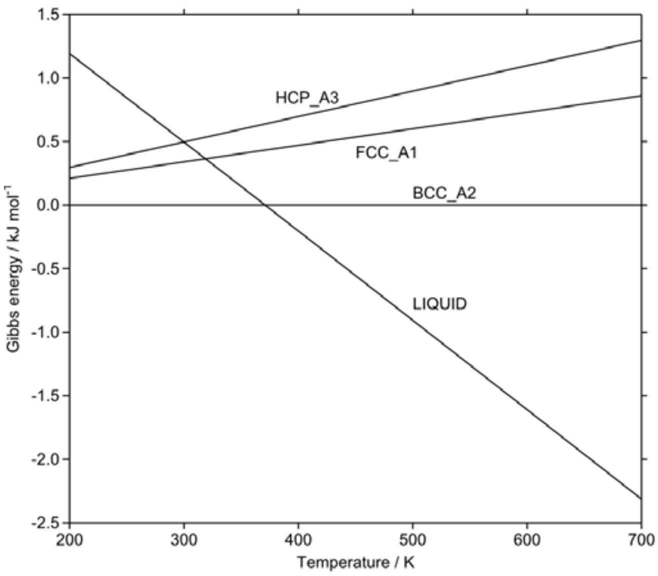
$-50 + 1.3\ T$ *(200 < T < 2300)*

HCP_A3

$-104 + 2\ T$ *(200 < T < 2300)*



Heat capacity of Na



Gibbs energy of phases of Na relative to BCC_A2

Nb

Source of data: *TPIS [BCC_A2, LIQUID]*
A Fernandez Guillermet, W Huang, Z. Metallkde., 1988, ***79****, 88-95, [FCC_A1, HCP_A3]*

BCC_A2

$-8519.353 + 142.045475\ T - 26.4711\ T\ \ln(T) + 0.203475E\text{-}3\ T^2 - 0.35012E\text{-}6\ T^3 + 93399\ T^{-1}$ *(298.15 < T < 2750)*

$-37669.3 + 271.720843\ T - 41.77\ T\ \ln(T) + 1528.238E29\ T^{-9}$ *(2750 < T < 6000)*

LIQUID

$21262.202 + 131.229057\ T - 26.4711\ T\ \ln(T) + 0.203475E\text{-}3\ T^2 - 0.35012E\text{-}6\ T^3 + 93399\ T^{-1} - 306.098E\text{-}25\ T^7$ *(298.15 < T < 2750)*

$-7499.398 + 260.756148\ T - 41.77\ T\ \ln(T)$ *(2750 < T < 6000)*

FCC_A1

$4980.647 + 143.745475\ T - 26.4711\ T\ \ln(T) + 0.203475E\text{-}3\ T^2 - 0.35012E\text{-}6\ T^3 + 93399\ T^{-1}$ *(298.15 < T < 2750)*

$-24169.3 + 273.420843\ T - 41.77\ T\ \ln(T) + 1528.238E29\ T^{-9}$ *(2750 < T < 6000)*

HCP_A3

$1480.647 + 144.445475\ T - 26.4711\ T\ \ln(T) + 0.203475E\text{-}3\ T^2 - 0.35012E\text{-}6\ T^3 + 93399\ T^{-1}$ *(298.15 < T < 2750)*

$-27669.3 + 274.120843\ T - 41.77\ T\ \ln(T) + 1528.238E29\ T^{-9}$ *(2750 < T < 6000)*

Data relative to BCC_A2

LIQUID

$29781.555 - 10.816418\ T - 306.098E\text{-}25\ T^7$ *(298.15 < T < 2750)*

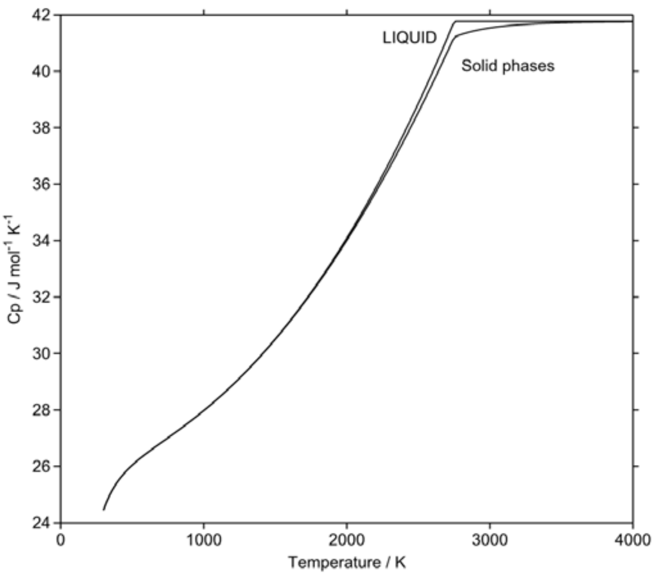
$30169.902 - 10.964695\ T - 1528.238E29\ T^{-9}$ *(2750 < T < 6000)*

FCC_A1

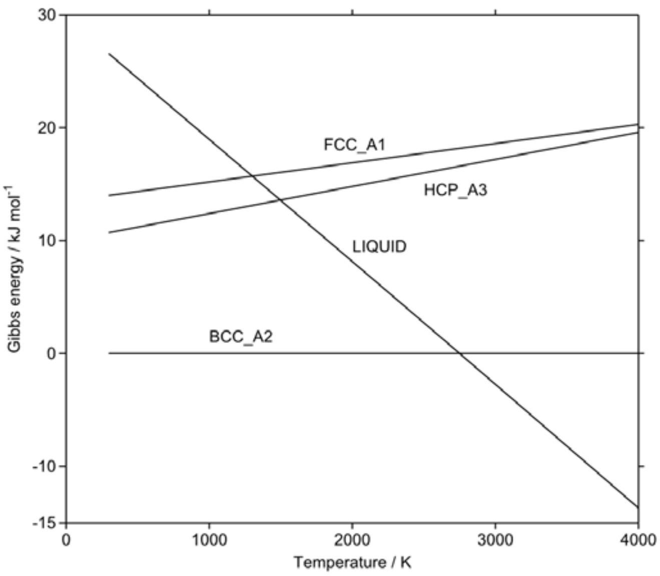
$13500 + 1.7\ T$ *(298.15 < T < 6000)*

HCP_A3

$10000 + 2.4\ T$ *(298.15 < T < 6000)*



Heat capacity of Nb



Gibbs energy of phases of Nb relative to BCC_A2

Nd

Source of data: *Hultgren extended by A T Dinsdale [DHCP, BCC_A2, LIQUID]*
S Norgren, Thesis, Royal Institute of Technology Stockholm, 2000 [HCP_A3]
G Cacciamani, G Borzone, R Ferro in COST507 Final report (COST507 Thermochemical database for light metal alloys, Volume 2 eds I Ansara, A T Dinsdale and M H Rand, July 1998, EUR18499) [FCC_A1]

DHCP

$-8402.93 + 111.10239\ T - 27.0858\ T\ln(T) + 0.556125E\text{-}3\ T^2 - 2.6923E\text{-}6\ T^3 + 34887\ T^{-1}$ *(298.15 < T < 900)*

$-6984.083 + 83.662617\ T - 22.7536\ T\ln(T) - 4.20402E\text{-}3\ T^2 - 1.802E\text{-}6\ T^3$ *(900 < T < 1128)*

$-225610.846 + 1673.040749\ T - 238.1828733\ T\ln(T) + 78.615997E\text{-}3\ T^2 - 6.048207E\text{-}6\ T^3 + 38810350\ T^{-1}$ *(1128 < T < 1799)*

$-25742.331 + 276.257088\ T - 48.7854\ T\ln(T)$ *(1799 < T < 1800)*

BCC_A2

$-6965.635 + 110.556109\ T - 27.0858\ T\ln(T) + 0.556125E\text{-}3\ T^2 - 2.6923E\text{-}6\ T^3 + 34887\ T^{-1}$ *(298.15 < T < 400)*

$7312.2 - 153.033976\ T + 14.9956777\ T\ln(T) - 50.479E\text{-}3\ T^2 + 7.287217E\text{-}6\ T^3 - 831810\ T^{-1}$ *(400 < T < 1128)*

$-18030.266 + 239.677322\ T - 44.5596\ T\ln(T)$ *(1128 < T < 1289)*

$334513.017 - 2363.919899\ T + 311.409193\ T\ln(T) - 156.030778E\text{-}3\ T^2 + 12.408421E\text{-}6\ T^3 - 64319604\ T^{-1}$ *(1289 < T < 1799)*

$-24495.579 + 274.879155\ T - 48.7854\ T\ln(T)$ *(1799 < T < 1800)*

LIQUID

$-3351.187 + 109.517314\ T - 27.0858\ T \ln(T) + 0.556125E\text{-}3\ T^2 - 2.6923E\text{-}6\ T^3 + 34887\ T^{-1}$
(298.15 < T < 300)

$5350.01 - 86.593963\ T + 5.357301\ T \ln(T) - 46.955463E\text{-}3\ T^2 + 6.860782E\text{-}6\ T^3 - 374380\ T^{-1}$
(300 < T < 1128)

$-16335.232 + 268.625903\ T - 48.7854\ T \ln(T)$ *(1128 < T < 1800)*

FCC_A1

$-7902.93 + 111.10239\ T - 27.0858\ T \ln(T) + 0.556125E\text{-}3\ T^2 - 2.6923E\text{-}6\ T^3 + 34887\ T^{-1}$
(298.15 < T < 900)

$-6484.083 + 83.662617\ T - 22.7536\ T \ln(T) - 4.20402E\text{-}3\ T^2 - 1.802E\text{-}6\ T^3$ *(900 < T < 1128)*

$-225110.846 + 1673.040749\ T - 238.1828733\ T \ln(T) + 78.615997E\text{-}3\ T^2 - 6.048207E\text{-}6\ T^3$
$+ 38810350\ T^{-1}$ *(1128 < T < 1799)*

$-25242.331 + 276.257088\ T - 48.7854\ T \ln(T)$ *(1799 < T < 1800)*

HCP_A3

$-6902.93 + 110.686665\ T - 27.0858\ T \ln(T) + 0.556125E\text{-}3\ T^2 - 2.6923E\text{-}6\ T^3 + 34887\ T^{-1}$
(298.15 < T < 900)

$-5484.083 + 83.246892\ T - 22.7536\ T \ln(T) - 4.20402E\text{-}3\ T^2 - 1.802E\text{-}6\ T^3$ *(900 < T < 1128)*

$-224110.846 + 1672.625024\ T - 238.1828733\ T \ln(T) + 78.615997E\text{-}3\ T^2 - 6.048207E\text{-}6\ T^3$
$+ 38810350\ T^{-1}$ *(1128 < T < 1799)*

$-24242.331 + 275.841363\ T - 48.7854\ T \ln(T)$ *(1799 < T < 1800)*

Data relative to DHCP

BCC_A2

$1437.295 - 0.546281\ T$ *(298.15 < T < 400)*

$15715.13 - 264.136366\ T + 42.0814777\ T \ln(T) - 51.035125E\text{-}3\ T^2 + 9.979517E\text{-}6\ T^3 - 866697\ T^{-1}$
(400 < T < 900)

$14296.283 - 236.696593\ T + 37.7492777\ T \ln(T) - 46.27498E\text{-}3\ T^2 + 9.089217E\text{-}6\ T^3 - 831810\ T^{-1}$
(900 < T < 1128)

$207580.58 - 1433.363427\ T + 193.6232733\ T \ln(T) - 78.615997E\text{-}3\ T^2 + 6.048207E\text{-}6\ T^3 - 38810350\ T^{-1}$
(1128 < T < 1289)

$560123.863 - 4036.960648\ T + 549.5920663\ T \ln(T) - 234.646775E\text{-}3\ T^2 + 18.456628E\text{-}6\ T^3$
$- 103129954\ T^{-1}$ *(1289 < T < 1799)*

$1246.752 - 1.377933\ T$ *(1799 < T < 1800)*

LIQUID

$5051.743 - 1.585076\ T$ *(298.15 < T < 300)*

$13752.94 - 197.696353\ T + 32.443101\ T \ln(T) - 47.511588E\text{-}3\ T^2 + 9.553082E\text{-}6\ T^3 - 409267\ T^{-1}$
(300 < T < 900)

$12334.093 - 170.25658\ T + 28.110901\ T\ \ln(T) - 42.751443E\text{-}3\ T^2 + 8.662782E\text{-}6\ T^3 - 374380\ T^{-1}$ *(900 < T < 1128)*

$209275.614 - 1404.414846\ T + 189.3974733\ T\ \ln(T) - 78.615997E\text{-}3\ T^2 + 6.048207E\text{-}6\ T^3$
$- 38810350\ T^{-1}$ *(1128 < T < 1799)*

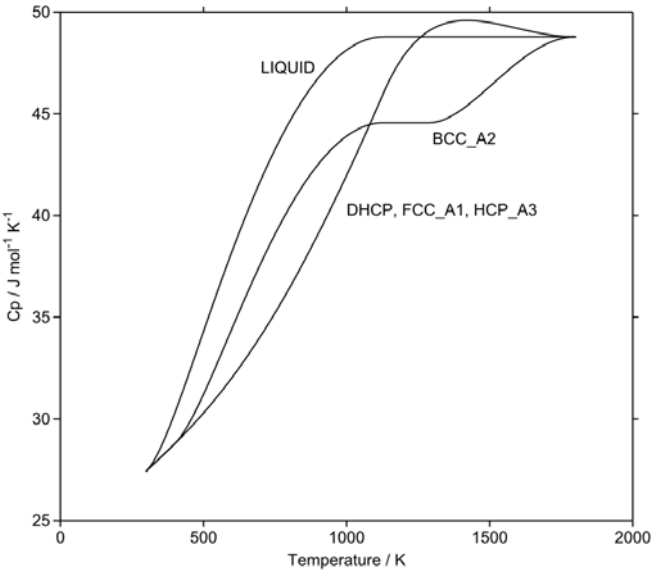
$9407.099 - 7.631185\ T$ *(1799 < T < 1800)*

FCC_A1

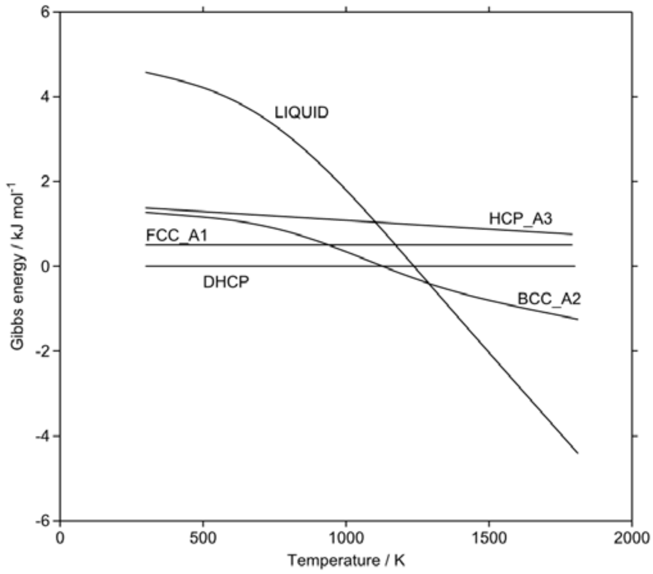
500 *(298.15 < T < 1800)*

HCP_A3

$1500 - 0.415725\ T$ *(298.15 < T < 1800)*



Heat capacity of Nd



Gibbs energy of phases of Nd relative to DHCP

Ni

Source of data: *A T Dinsdale, unpublished work [FCC_A1, LIQUID, BCC_A2]*
*A Fernandez Guillermet, Z. Metallkde., 1987, **78**, 639-47 [HCP_A3]*
Kaufman [BCC_A12, CUB_A13]
G Ghosh; Metall. Mater. Trans. A, 1999, 30A(6), 1481-1494 [BCT_A5]

FCC_A1

$T_C = 633$ $B_0 = 0.52$
$A = 6.533939E\text{-}6$ $a_0 = 3.103614E\text{-}5$ $a_1 = 2.418404E\text{-}8$
$K_0 = 5.3297107E\text{-}12$ $K_1 = 4.5132279E\text{-}16$ $K_2 = 9.7669517E\text{-}19$ $n = 4.651$

$-5179.159 + 117.854\ T - 22.096\ T\ \ln(T) - 4.8407E\text{-}3\ T^2 + Gpres + Gmag$ *(298.15 < T < 1728)*

$-27840.620 + 279.134977\ T - 43.1\ T\ \ln(T) + 1127.54E28\ T^{-9} + Gpres + Gmag$ *(1728 < T < 3000)*

LIQUID

$11235.527 + 108.457\ T - 22.096\ T\ln(T) - 4.8407E\text{-}3\ T^2 - 382.318E\text{-}23\ T^7$ *(298.15 < T < 1728)*
$-9549.817 + 268.597977\ T - 43.1\ T\ln(T)$ *(1728 < T < 3000)*

BCC_A2

$T_C = 575$ $B_0 = 0.85$

$3535.925 + 114.298\ T - 22.096\ T\ln(T) - 4.8407E\text{-}3\ T^2 + Gmag$ *(298.15 < T < 1728)*
$-19125.536 + 275.578977\ T - 43.1\ T\ln(T) + 1127.54E28\ T^{-9} + Gmag$ *(1728 < T < 3000)*

CBCC_A12

$-1623.159 + 117.854\ T - 22.096\ T\ln(T) - 4.8407E\text{-}3\ T^2$ *(298.15 < T < 1728)*
$-24284.620 + 279.134977\ T - 43.1\ T\ln(T) + 1127.54E28\ T^{-9}$ *(1728 < T < 3000)*

CUB_A13

$-3087.159 + 117.854\ T - 22.096\ T\ln(T) - 4.8407E\text{-}3\ T^2$ *(298.15 < T < 1728)*
$-25748.620 + 279.134977\ T - 43.1\ T\ln(T) + 1127.54E28\ T^{-9}$ *(1728 < T < 3000)*

HCP_A3

$T_C = 633$ $B_0 = 0.52$

$-4133.159 + 119.1092\ T - 22.096\ T\ln(T) - 4.8407E\text{-}3\ T^2 + Gmag$ *(298.15 < T < 1728)*
$-26794.620 + 280.390177\ T - 43.1\ T\ln(T) + 1127.54E28\ T^{-9} + Gmag$ *(1728 < T < 3000)*

BCT_A5

$4843.841 + 113.298\ T - 22.096\ T\ln(T) - 4.8407E\text{-}3\ T^2$ *(298.15 < T < 1728)*
$-17817.62 + 274.578977\ T - 43.1\ T\ln(T) + 1127.54E28\ T^{-9}$ *(1728 < T < 3000)*

Data relative to paramagnetic FCC_A1

FCC_A1

$T_C = 633$ $B_0 = 0.52$
$A = 6.533939E\text{-}6$ $a_0 = 3.103614E\text{-}5$ $a_1 = 2.418404E\text{-}8$
$K_0 = 5.3297107E\text{-}12$ $K_1 = 4.5132279E\text{-}16$ $K_2 = 9.7669517E\text{-}19$ $n = 4.651$

$Gmag + Gpres$ *(298.15 < T < 3000)*

LIQUID

$16414.686 - 9.397\ T - 382.318E\text{-}23\ T^7$ *(298.15 < T < 1728)*
$18290.803 - 10.537\ T - 1127.54E28\ T^{-9}$ *(1728 < T < 3000)*

BCC_A2

$T_C = 575$ $B_0 = 0.85$

8715.084 - 3.556 T + Gmag *(298.15 < T < 3000)*

CBCC_A12

3556 *(298.15 < T < 3000)*

CUB_A13

2092 *(298.15 < T < 3000)*

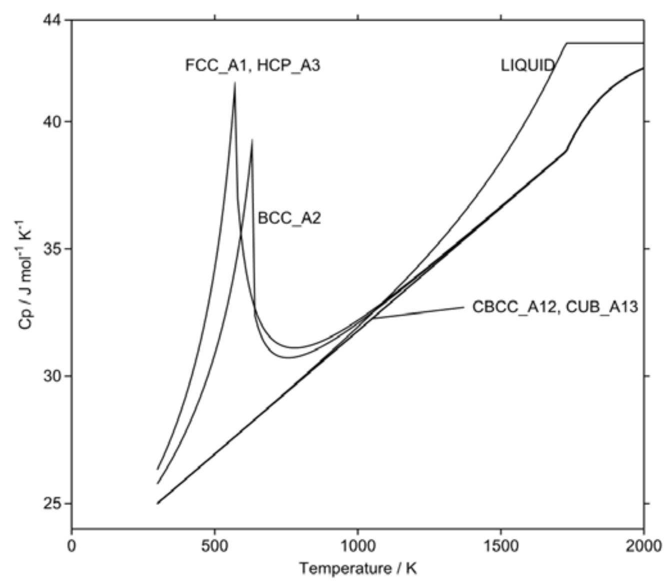
HCP_A3

$T_C = 633$ $B_0 = 0.52$

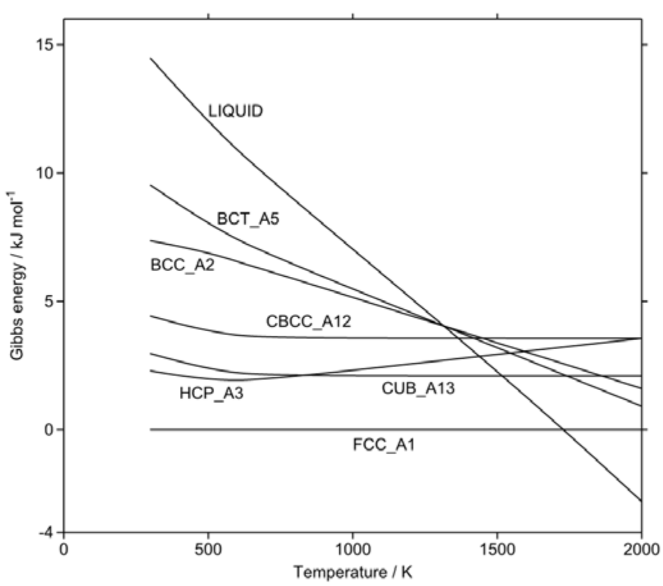
1046 + 1.2552 T + Gmag *(298.15 < T < 3000)*

BCT_A5

10023 - 4.556 T *(298.15 < T < 3000)*



Heat capacity of Ni



Gibbs energy of phases of Ni relative to FCC_A1

Np

Source of data: *M H Rand (Unpublished work)*

ORTHO_Ac

$241.888 - 57.531347 T + 4.0543 T \ln(T) - 41.27725E-3 T^2 - 402857 T^{-1}$ *(298.15 < T < 553)*
$-57015.112 + 664.27337 T - 102.523 T \ln(T) + 28.4592E-3 T^2 - 2.483917E-6 T^3 + 4796910 T^{-1}$
(553 < T < 1799)
$-12092.736 + 255.780866 T - 45.3964 T \ln(T)$ *(1799 < T < 4000)*

LIQUID

$-4627.18 + 160.024959 T - 31.229 T \ln(T) - 16.3885E-3 T^2 + 2.941883E-6 T^3 + 439915 T^{-1}$
(298.15 < T < 917)
$-7415.255 + 247.671446 T - 45.3964 T \ln(T)$ *(917 < T < 4000)*

TETRAG_Ad

$-10157.32 + 183.829213 T - 34.11 T \ln(T) - 16.1186E-3 T^2 + 4.98465E-6 T^3 + 532825 T^{-1}$
(298.15 < T < 555)
$-7873.688 + 207.01896 T - 39.33 T \ln(T)$ *(555 < T < 856)*
$19027.98 - 46.64846 T - 3.4265 T \ln(T) - 19.21045E-3 T^2 + 1.52726E-6 T^3 - 3564640 T^{-1}$
(856 < T < 1999)
$-16070.82 + 256.707037 T - 45.3964 T \ln(T)$ *(1999 < T < 4000)*

BCC_A2

$-3224.664 + 174.911817 T - 35.177 T \ln(T) - 2.51865E-3 T^2 + 0.514743E-6 T^3 + 302225 T^{-1}$
(298.15 < T < 856)
$-2366.486 + 180.807719 T - 36.401 T \ln(T)$ *(856 < T < 917)*
$50882.281 - 297.324358 T + 30.7734 T \ln(T) - 34.3483E-3 T^2 + 2.707217E-6 T^3 - 7500100 T^{-1}$
(917 < T < 1999)
$-14879.686 + 254.773087 T - 45.3964 T \ln(T)$ *(1999 < T < 4000)*

Data relative to ORTHO_Ac

LIQUID

$-4869.068 + 217.556306 T - 35.2833 T \ln(T) + 24.88875E-3 T^2 + 2.941883E-6 T^3 + 842772 T^{-1}$
(298.15 < T < 553)
$52387.932 - 504.248411 T + 71.294 T \ln(T) - 44.8477E-3 T^2 + 5.4258E-6 T^3 - 4356995 T^{-1}$
(553 < T < 917)
$49599.857 - 416.601924 T + 57.1266 T \ln(T) - 28.4592E-3 T^2 + 2.483917E-6 T^3 - 4796910 T^{-1}$
(917 < T < 1799)
$4677.481 - 8.10942 T$ *(1799 < T < 4000)*

TETRAG_Ad

$-10399.208 + 241.36056\ T - 38.1643\ T\ \ln(T) + 25.15865E\text{-}3\ T^2 + 4.98465E\text{-}6\ T^3 + 935682\ T^{-1}$ *(298.15 < T < 553)*

$46857.792 - 480.444157\ T + 68.413\ T\ \ln(T) - 44.5778E\text{-}3\ T^2 + 7.468567E\text{-}6\ T^3 - 4264085\ T^{-1}$ *(553 < T < 555)*

$49141.424 - 457.25441\ T + 63.193\ T\ \ln(T) - 28.4592E\text{-}3\ T^2 + 2.483917E\text{-}6\ T^3 - 4796910\ T^{-1}$ *(555 < T < 856)*

$76043.092 - 710.92183\ T + 99.0965\ T\ \ln(T) - 47.66965E\text{-}3\ T^2 + 4.011177E\text{-}6\ T^3 - 8361550\ T^{-1}$ *(856 < T < 1799)*

$31120.716 - 302.429326\ T + 41.9699\ T\ \ln(T) - 19.21045E\text{-}3\ T^2 + 1.52726E\text{-}6\ T^3 - 3564640\ T^{-1}$ *(1799 < T < 1999)*

$-3978.084 + 0.926171\ T$ *(1999 < T < 4000)*

BCC_A2

$-3466.552 + 232.443164\ T - 39.2313\ T\ \ln(T) + 38.7586E\text{-}3\ T^2 + 0.514743E\text{-}6\ T^3 + 705082\ T^{-1}$ *(298.15 < T < 553)*

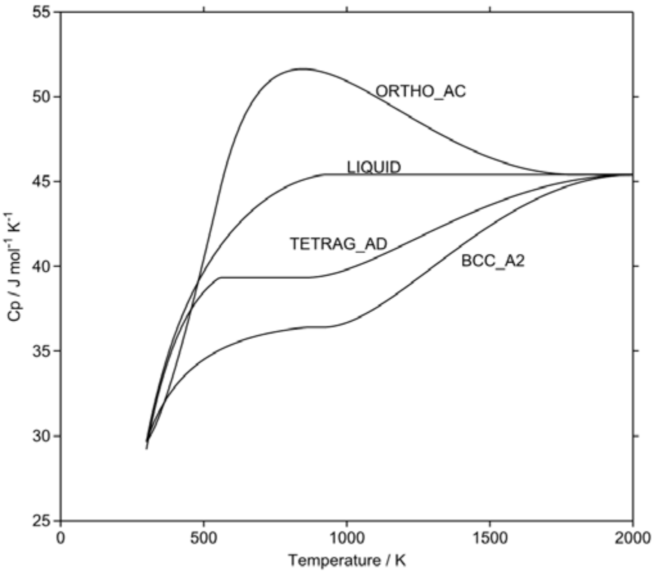
$53790.448 - 489.361553\ T + 67.346\ T\ \ln(T) - 30.97785E\text{-}3\ T^2 + 2.99866E\text{-}6\ T^3 - 4494685\ T^{-1}$ *(553 < T < 856)*

$54648.626 - 483.465651\ T + 66.122\ T\ \ln(T) - 28.4592E\text{-}3\ T^2 + 2.483917E\text{-}6\ T^3 - 4796910\ T^{-1}$ *(856 < T < 917)*

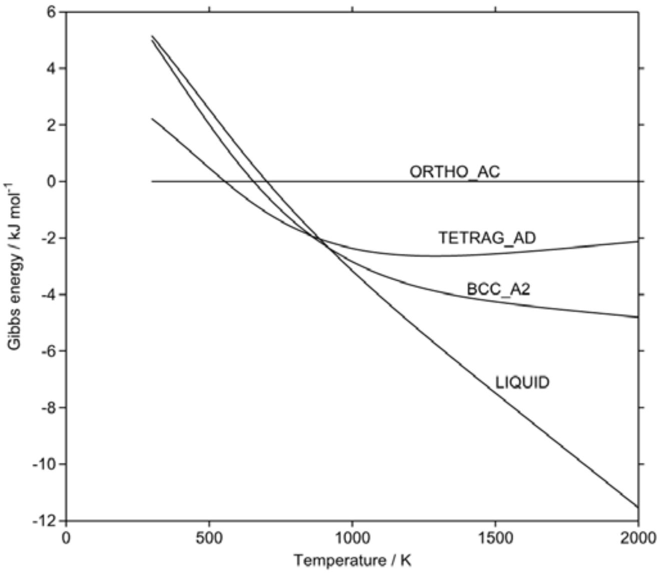
$107897.393 - 961.597728\ T + 133.2964\ T\ \ln(T) - 62.8075E\text{-}3\ T^2 + 5.191134E\text{-}6\ T^3 - 12297010\ T^{-1}$ *(917 < T < 1799)*

$62975.017 - 553.105224\ T + 76.1698\ T\ \ln(T) - 34.3483E\text{-}3\ T^2 + 2.707217E\text{-}6\ T^3 - 7500100\ T^{-1}$ *(1799 < T < 1999)*

$-2786.95 - 1.007779\ T$ *(1999 < T < 4000)*



Heat capacity of Np



Gibbs energy of phases of Np relative to ORTHO_Ac

O

Source of data: *JANAF [GAS]*
*R Schmidt, Metall. Trans., 1983, **14B**, 473-81 [LIQUID]*
*B Sundman, J. Phase Equil., 1991, **12**(1), 127-40 [BCC_A2, FCC_A1]*

GAS (1/2O2<g>)

$-3480.87 - 25.503038\ T - 11.1355\ T\ln(T) - 5.098875E{-3}\ T^2 + 0.661846E{-6}\ T^3 - 38365\ T^{-1}$
(298.15 < T < 1000)
$-6568.763 + 12.659879\ T - 16.8138\ T\ln(T) - 0.595797E{-3}\ T^2 + 0.006781E{-6}\ T^3 + 262905\ T^{-1}$
(1000 < T < 3300)
$-13986.728 + 31.259624\ T - 18.9536\ T\ln(T) - 0.425243E{-3}\ T^2 + 0.010721E{-6}\ T^3 + 4383200\ T^{-1}$
(3300 < T < 6000)

LIQUID

$-6129.77 + 5.936962\ T - 11.1355\ T\ln(T) - 5.098875E{-3}\ T^2 + 0.661846E{-6}\ T^3 - 38365\ T^{-1}$
(298.15 < T < 1000)
$-9217.663 + 44.099879\ T - 16.8138\ T\ln(T) - 0.595797E{-3}\ T^2 + 0.006781E{-6}\ T^3 + 262905\ T^{-1}$
(1000 < T < 3300)
$-16635.628 + 62.699624\ T - 18.9536\ T\ln(T) - 0.425243E{-3}\ T^2 + 0.010721E{-6}\ T^3 + 4383200\ T^{-1}$
(3300 < T < 6000)

BCC_A2

$26519.13 - 25.503038\ T - 11.1355\ T\ln(T) - 5.098875E{-3}\ T^2 + 0.661846E{-6}\ T^3 - 38365\ T^{-1}$
(298.15 < T < 1000)
$23431.237 + 12.659879\ T - 16.8138\ T\ln(T) - 0.595797E{-3}\ T^2 + 0.006781E{-6}\ T^3 + 262905\ T^{-1}$
(1000 < T < 3300)
$16013.272 + 31.259624\ T - 18.9536\ T\ln(T) - 0.425243E{-3}\ T^2 + 0.010721E{-6}\ T^3 + 4383200\ T^{-1}$
(3300 < T < 6000)

FCC_A1

$26519.13 - 25.503038\ T - 11.1355\ T\ln(T) - 5.098875E{-3}\ T^2 + 0.661846E{-6}\ T^3 - 38365\ T^{-1}$
(298.15 < T < 1000)
$23431.237 + 12.659879\ T - 16.8138\ T\ln(T) - 0.595797E{-3}\ T^2 + 0.006781E{-6}\ T^3 + 262905\ T^{-1}$
(1000 < T < 3300)
$16013.272 + 31.259624\ T - 18.9536\ T\ln(T) - 0.425243E{-3}\ T^2 + 0.010721E{-6}\ T^3 + 4383200\ T^{-1}$
(3300 < T < 6000)

Data relative to 0.5O2<GAS>

LIQUID

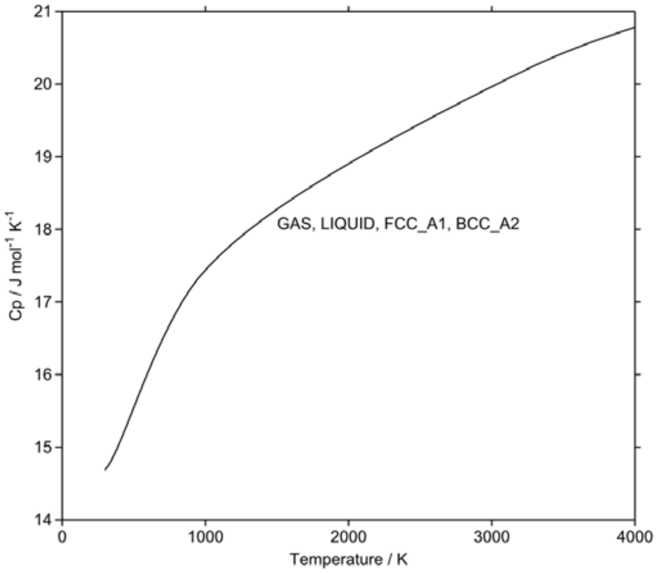
$-2648.9 + 31.44\ T$ *(298.15 < T < 6000)*

BCC_A2

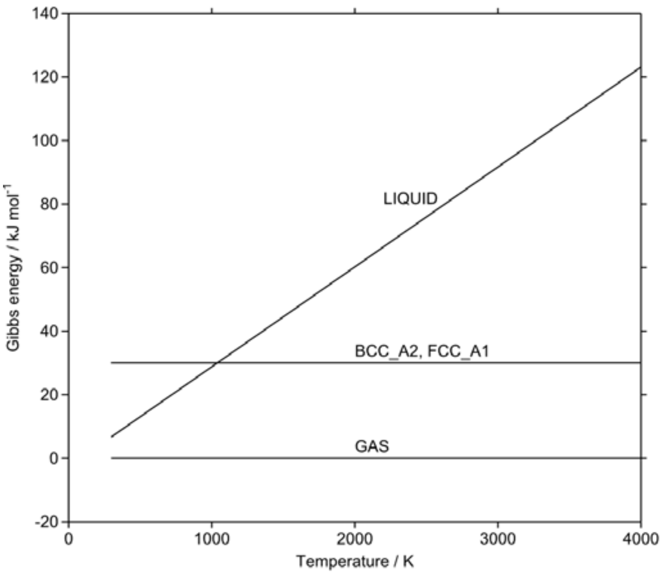
30000 *(298.15 < T < 6000)*

FCC_A1

30000 *(298.15 < T < 6000)*



Heat capacity of O



Gibbs energy of phases of O relative to GAS

Os

Source of data: *Hultgren [HCP_A3]*
Saunders et al. [LIQUID, FCC_A1, BCC_A2]

HCP_A3

$-7196.978 + 126.369531\ T - 23.5710242\ T\ \ln(T) - 1.90427E\text{-}3\ T^2$ *(298.15 < T < 3306)*
$644910.07 - 1935.213696\ T + 224.9980343\ T\ \ln(T) - 42.489827E\text{-}3\ T^2 + 1.173861E\text{-}6\ T^3$
$- 312569031\ T^{-1}$ *(3306 < T < 5500)*

LIQUID

$29263.192 + 117.895788\ T - 23.5710242\ T\ \ln(T) - 1.90427E\text{-}3\ T^2$ *(298.15 < T < 1000)*
$68715.318 - 198.324341\ T + 19.9382156\ T\ \ln(T) - 20.464464E\text{-}3\ T^2 + 1.014279E\text{-}6\ T^3 - 6237261\ T^{-1}$
(1000 < T < 3306)
$-15903.192 + 336.874526\ T - 50\ T\ \ln(T)$ *(3306 < T < 5500)*

BCC_A2

20303.022 + 121.969531 T - 23.5710242 T ln(T) - 1.90427E-3 T^2 *(298.15 < T < 3306)*
672410.07 - 1939.613696 T + 224.9980343 T ln(T) - 42.489827E-3 T^2 + 1.173861E-6 T^3
 - 312569031 T^{-1} *(3306 < T < 5500)*

FCC_A1

5803.022 + 123.869531 T - 23.5710242 T ln(T) - 1.90427E-3 T^2 *(298.15 < T < 3306)*
657910.07 - 1937.713696 T + 224.9980343 T ln(T) - 42.489827E-3 T^2 + 1.173861E-6 T^3
 - 312569031 T^{-1} *(3306 < T < 5500)*

Data relative to HCP_A3

LIQUID

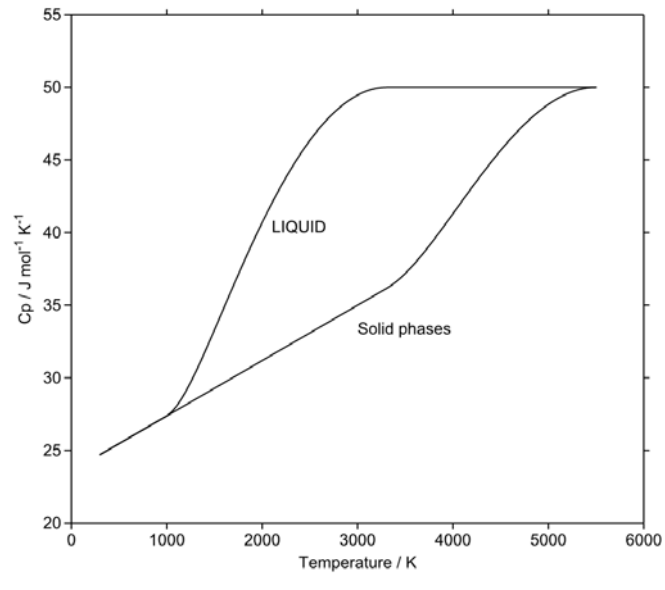
36460.17 - 8.473743 T *(298.15 < T < 1000)*
75912.296 - 324.693872 T + 43.5092398 T ln(T) - 18.560194E-3 T^2 + 1.014279E-6 T^3 - 6237261 T^{-1}
(1000 < T < 3306)
-660813.262 + 2272.088222 T - 274.9980343 T ln(T) + 42.489827E-3 T^2 - 1.173861E-6 T^3
 + 312569031 T^{-1} *(3306 < T < 5500)*

BCC_A2

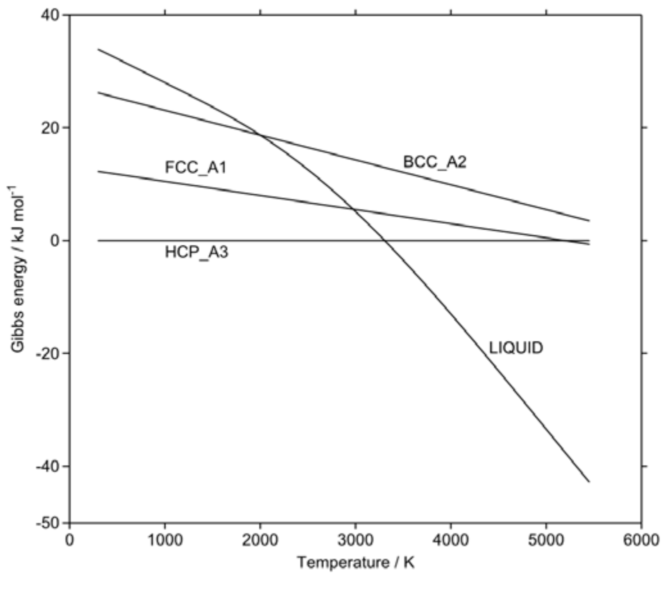
27500 - 4.4 T *(298.15 < T < 5500)*

FCC_A1

13000 - 2.5 T *(298.15 < T < 5500)*



Heat capacity of Os



Gibbs energy of phases of Os relative to HCP_A3

P

Source of data: *JANAF [WHITE_P, RED_P, LIQUID]*
B Uhrenius (unpublished work) [BCC_A2]
Kaufman [FCC_A1]
Note: *By convention the WHITE_P form is taken as reference phase although the RED_P is very much more stable.*

WHITE_P

$-43821.799 + 1026.693886\ T - 178.426\ T \ln(T) + 290.708E\text{-}3\ T^2 - 104.022667E\text{-}6\ T^3 + 1632695\ T^{-1}$ *(250 < T < 317.3)*

$-9587.448 + 152.341487\ T - 28.7335301\ T \ln(T) + 1.715669E\text{-}3\ T^2 - 0.22829E\text{-}6\ T^3 + 172966\ T^{-1}$ *(317.3 < T < 1000)*

$-8093.075 + 135.876831\ T - 26.326\ T \ln(T)$ *(1000 < T < 3000)*

RED_P

$-25976.559 + 148.672002\ T - 25.55\ T \ln(T) + 3.4121E\text{-}3\ T^2 - 2.418867E\text{-}6\ T^3 + 160095\ T^{-1}$ *(250 < T < 500)*

$-21723.721 + 77.671737\ T - 14.368\ T \ln(T) - 9.57685E\text{-}3\ T^2 + 0.393917E\text{-}6\ T^3 - 141375\ T^{-1}$ *(500 < T < 852.35)*

$-119408.413 + 1026.02962\ T - 149.4495562\ T \ln(T) + 67.272364E\text{-}3\ T^2 - 6.651929E\text{-}6\ T^3 + 12495943\ T^{-1}$ *(852.35 < T < 1500)*

$-24524.119 + 153.839181\ T - 26.326\ T \ln(T)$ *(1500 < T < 3000)*

LIQUID

$-26316.111 + 434.930931\ T - 70.7440584\ T \ln(T) - 2.898936E\text{-}3\ T^2 + 39.049371E\text{-}6\ T^3 + 1141147\ T^{-1}$ *(250 < T < 317.3)*

$-7232.449 + 133.291873\ T - 26.326\ T \ln(T)$ *(317.3 < T < 3000)*

RHOMBOHEDRAL_A7

$-44009.799 + 1026.819156\ T - 178.426\ T \ln(T) + 290.708E\text{-}3\ T^2 - 104.022667E\text{-}6\ T^3 + 1632695\ T^{-1}$ *(250 < T < 317.3)*

$-9775.448 + 152.466757\ T - 28.7335301\ T \ln(T) + 1.715669E\text{-}3\ T^2 - 0.22829E\text{-}6\ T^3 + 172966\ T^{-1}$ *(317.3 < T < 1000)*

$-8281.075 + 136.002101\ T - 26.326\ T \ln(T)$ *(1000 < T < 3000)*

BCC_A2

$18792.241 + 135.412002\ T - 25.55\ T \ln(T) + 3.4121E\text{-}3\ T^2 - 2.418867E\text{-}6\ T^3 + 160095\ T^{-1}$ *(250 < T < 500)*

$23045.079 + 64.411737\ T - 14.368\ T \ln(T) - 9.57685E\text{-}3\ T^2 + 0.393917E\text{-}6\ T^3 - 141375\ T^{-1}$ *(500 < T < 852.35)*

$-74639.613 + 1012.76962\,T - 149.4495562\,T\ln(T) + 67.272364E{-3}\,T^2 - 6.651929E{-6}\,T^3 + 12495943\,T^{-1}$

(852.35 < T < 1500)

$20244.681 + 140.579181\,T - 26.326\,T\ln(T)$ *(1500 < T < 3000)*

FCC_A1

$10842.441 + 135.534002\,T - 25.55\,T\ln(T) + 3.4121E{-3}\,T^2 - 2.418867E{-6}\,T^3 + 160095\,T^{-1}$

(250 < T < 500)

$15095.279 + 64.533737\,T - 14.368\,T\ln(T) - 9.57685E{-3}\,T^2 + 0.393917E{-6}\,T^3 - 141375\,T^{-1}$

(500 < T < 852.35)

$-82589.413 + 1012.89162\,T - 149.4495562\,T\ln(T) + 67.272364E{-3}\,T^2 - 6.651929E{-6}\,T^3 + 12495943\,T^{-1}$

(852.35 < T < 1500)

$12294.881 + 140.701181\,T - 26.326\,T\ln(T)$ *(1500 < T < 3000)*

Data relative to WHITE_P

RED_P

$17845.24 - 878.021884\,T + 152.876\,T\ln(T) - 287.2959E{-3}\,T^2 + 101.6038E{-6}\,T^3 - 1472600\,T^{-1}$

(250 < T < 317.3)

$-16389.111 - 3.669485\,T + 3.1835301\,T\ln(T) + 1.696431E{-3}\,T^2 - 2.190577E{-6}\,T^3 - 12871\,T^{-1}$

(317.3 < T < 500)

$-12136.273 - 74.66975\,T + 14.3655301\,T\ln(T) - 11.292519E{-3}\,T^2 + 0.622207E{-6}\,T^3 - 314341\,T^{-1}$

(500 < T < 852.35)

$-109820.965 + 873.688133\,T - 120.7160261\,T\ln(T) + 65.556695E{-3}\,T^2 - 6.423639E{-6}\,T^3$
$+ 12322977\,T^{-1}$ *(852.35 < T < 1000)*

$-111315.338 + 890.152789\,T - 123.1235562\,T\ln(T) + 67.272364E{-3}\,T^2 - 6.651929E{-6}\,T^3$
$+ 12495943\,T^{-1}$ *(1000 < T < 1500)*

$-16431.044 + 17.96235\,T$ *(1500 < T < 3000)*

LIQUID

$17505.688 - 591.762955\,T + 107.6819416\,T\ln(T) - 293.606936E{-3}\,T^2 + 143.072038E{-6}\,T^3 - 491548\,T^{-1}$

(250 < T < 317.3)

$2354.999 - 19.049614\,T + 2.4075301\,T\ln(T) - 1.715669E{-3}\,T^2 + 0.22829E{-6}\,T^3 - 172966\,T^{-1}$

(317.3 < T < 1000)

$860.626 - 2.584958\,T$ *(1000 < T < 3000)*

RHOMBOHEDRAL_A7

$-188 + 0.12527\,T$ *(250 < T < 3000)*

BCC_A2

$62614.04 - 891.281884\,T + 152.876\,T\ln(T) - 287.2959E{-3}\,T^2 + 101.6038E{-6}\,T^3 - 1472600\,T^{-1}$

(250 < T < 317.3)

$28379.689 - 16.929485\,T + 3.1835301\,T\ln(T) + 1.696431\text{E-}3\,T^2 - 2.190577\text{E-}6\,T^3 - 12871\,T^{-1}$

(317.3 < T < 500)

$32632.527 - 87.92975\,T + 14.3655301\,T\ln(T) - 11.292519\text{E-}3\,T^2 + 0.622207\text{E-}6\,T^3 - 314341\,T^{-1}$

(500 < T < 852.35)

$-65052.165 + 860.428133\,T - 120.7160261\,T\ln(T) + 65.556695\text{E-}3\,T^2 - 6.423639\text{E-}6\,T^3 + 12322977\,T^{-1}$

(852.35 < T < 1000)

$-66546.538 + 876.892789\,T - 123.1235562\,T\ln(T) + 67.272364\text{E-}3\,T^2 - 6.651929\text{E-}6\,T^3 + 12495943\,T^{-1}$

(1000 < T < 1500)

$28337.756 + 4.70235\,T$ *(1500 < T < 3000)*

FCC_A1

$54664.24 - 891.159884\,T + 152.876\,T\ln(T) - 287.2959\text{E-}3\,T^2 + 101.6038\text{E-}6\,T^3 - 1472600\,T^{-1}$

(250 < T < 317.3)

$20429.889 - 16.807485\,T + 3.1835301\,T\ln(T) + 1.696431\text{E-}3\,T^2 - 2.190577\text{E-}6\,T^3 - 12871\,T^{-1}$

(317.3 < T < 500)

$24682.727 - 87.80775\,T + 14.3655301\,T\ln(T) - 11.292519\text{E-}3\,T^2 + 0.622207\text{E-}6\,T^3 - 314341\,T^{-1}$

(500 < T < 852.35)

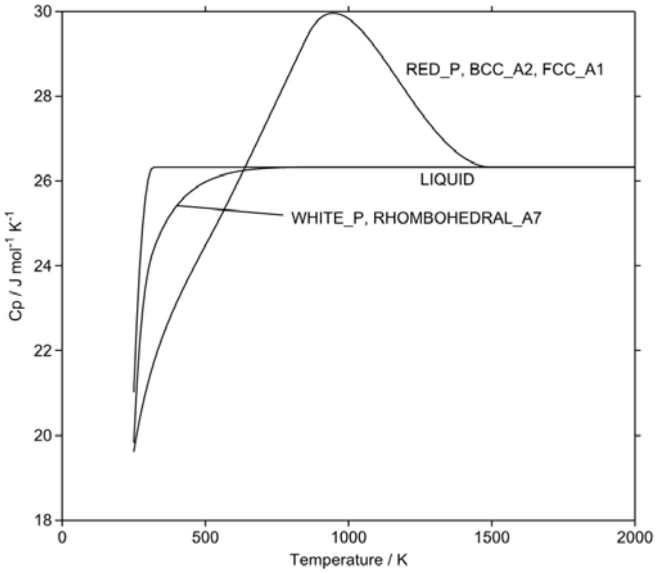
$-73001.965 + 860.550133\,T - 120.7160261\,T\ln(T) + 65.556695\text{E-}3\,T^2 - 6.423639\text{E-}6\,T^3 + 12322977\,T^{-1}$

(852.35 < T < 1000)

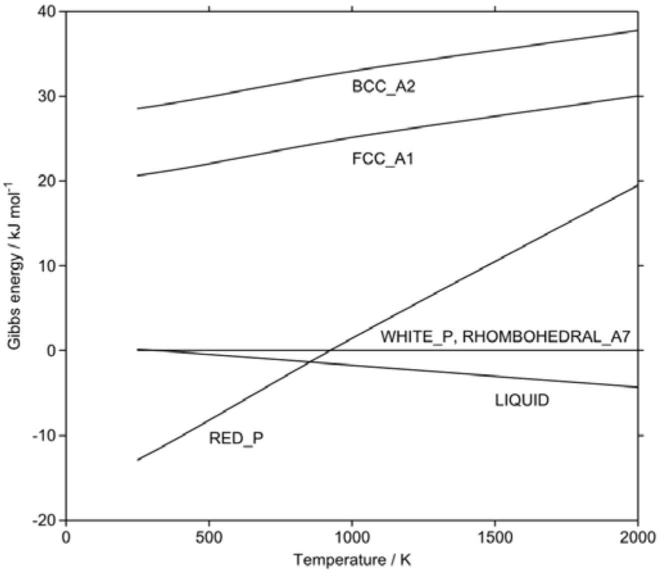
$-74496.338 + 877.014789\,T - 123.1235562\,T\ln(T) + 67.272364\text{E-}3\,T^2 - 6.651929\text{E-}6\,T^3 + 12495943\,T^{-1}$

(1000 < T < 1500)

$20387.956 + 4.82435\,T$ *(1500 < T < 3000)*



Heat capacity of P



Gibbs energy of phases of P relative to WHITE_P

Pa

Source of data: *M H Rand, Unpublished work*

BCT_Aa

$-7681.561 + 111.973215\ T - 23.9116\ T\ \ln(T) - 6.21325E\text{-}3\ T^2$ *(298.15 < T < 1443)*

$27955.763 - 177.320253\ T + 16.305\ T\ \ln(T) - 26.3416E\text{-}3\ T^2 + 1.884933E\text{-}6\ T^3 - 5908900\ T^{-1}$ *(1443 < T < 2176)*

$-29949.683 + 288.308639\ T - 47.2792\ T\ \ln(T)$ *(2176 < T < 4000)*

BCC_A2

$781.847 + 71.957409\ T - 18.203\ T\ \ln(T) - 13.22095E\text{-}3\ T^2 + 1.337387E\text{-}6\ T^3 - 101600\ T^{-1}$ *(298.15 < T < 1443)*

$-10955.948 + 220.478519\ T - 39.748\ T\ \ln(T)$ *(1443 < T < 1845)*

$284495.194 - 1397.150521\ T + 171.108\ T\ \ln(T) - 63.7105E\text{-}3\ T^2 + 3.343867E\text{-}6\ T^3 - 74992000\ T^{-1}$ *(1845 < T < 2710)*

$-27885.171 + 286.096187\ T - 47.2792\ T\ \ln(T)$ *(2710 < T < 4000)*

LIQUID

$8499.539 + 102.429215\ T - 23.9116\ T\ \ln(T) - 6.21325E\text{-}3\ T^2$ *(298.15 < T < 1088)*

$48013.96 - 278.789916\ T + 30.336\ T\ \ln(T) - 37.2478E\text{-}3\ T^2 + 3.075017E\text{-}6\ T^3 - 5064250\ T^{-1}$ *(1088 < T < 1845)*

$-12508.174 + 277.955437\ T - 47.2792\ T\ \ln(T)$ *(1845 < T < 4000)*

Data relative to BCT_Aa

BCC_A2

$8463.408 - 40.015806\ T + 5.7086\ T\ \ln(T) - 7.0077E\text{-}3\ T^2 + 1.337387E\text{-}6\ T^3 - 101600\ T^{-1}$ *(298.15 < T < 1443)*

$-38911.711 + 397.798772\ T - 56.053\ T\ \ln(T) + 26.3416E\text{-}3\ T^2 - 1.884933E\text{-}6\ T^3 + 5908900\ T^{-1}$ *(1443 < T < 1845)*

$256539.431 - 1219.830268\ T + 154.803\ T\ \ln(T) - 37.3689E\text{-}3\ T^2 + 1.458934E\text{-}6\ T^3 - 69083100\ T^{-1}$ *(1845 < T < 2176)*

$314444.877 - 1685.45916\ T + 218.3872\ T\ \ln(T) - 63.7105E\text{-}3\ T^2 + 3.343867E\text{-}6\ T^3 - 74992000\ T^{-1}$ *(2176 < T < 2710)*

$2064.512 - 2.212452\ T$ *(2710 < T < 4000)*

LIQUID

$16181.1 - 9.544\ T$ *(298.15 < T < 1088)*

$55695.521 - 390.763131\ T + 54.2476\ T\ \ln(T) - 31.03455E\text{-}3\ T^2 + 3.075017E\text{-}6\ T^3 - 5064250\ T^{-1}$ *(1088 < T < 1443)*

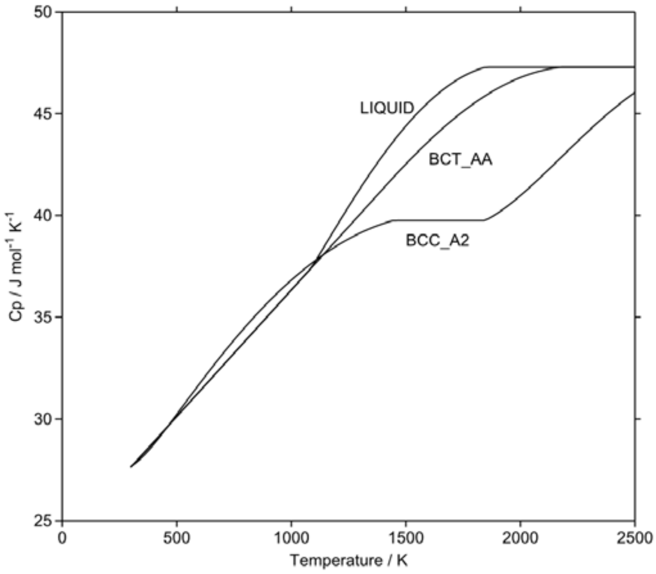
$20058.197 - 101.469663\ T + 14.031\ T\ln(T) - 10.9062E{-3}\ T^2 + 1.190084E{-6}\ T^3 + 844650\ T^{-1}$

(1443 < T < 1845)

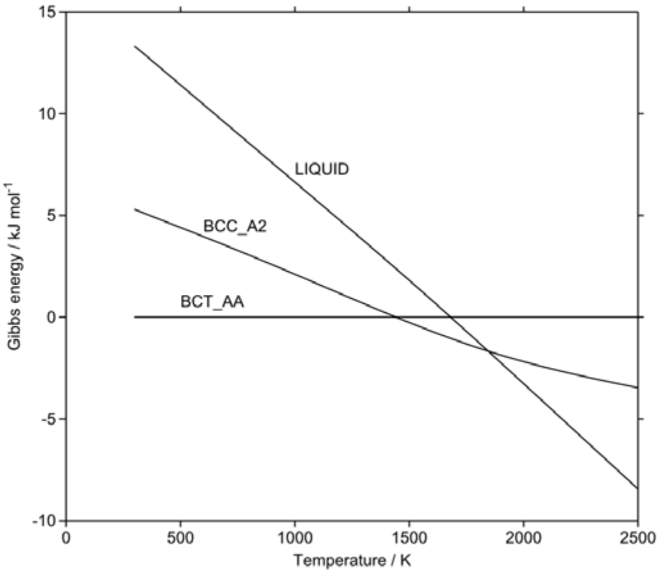
$-40463.937 + 455.27569\ T - 63.5842\ T\ln(T) + 26.3416E{-3}\ T^2 - 1.884933E{-6}\ T^3 + 5908900\ T^{-1}$

(1845 < T < 2176)

$17441.509 - 10.353202\ T$ *(2176 < T < 4000)*



Heat capacity of Pa



Gibbs energy of phases of Pa relative to BCT_Aa

Pb

Source of data: *JANAF [FCC_A1, LIQUID]*
T L Ngai, Y A Chang, CALPHAD, 1981, ***5****, 267 [BCT_A5]*
Saunders et al. [HCP_A3, BCC_A2]
D Boa, I Ansara, Thermochimica Acta 1998, 314, 79-86 [TET_ALPHA1, TETRAGONAL_A6, RHOMBOHEDRAL_A7]
A Maitre; J M Fiorani, M Vilasi, J Phase Equilib; 2002, 23(4), 329 [RHOMBO_A10]

FCC_A1

$-7650.085 + 101.700244\ T - 24.5242231\ T\ln(T) - 3.65895E{-3}\ T^2 - 0.24395E{-6}\ T^3$

(298.15 < T < 600.61)

$-10531.095 + 154.243182\ T - 32.4913959\ T\ln(T) + 1.54613E{-3}\ T^2 + 805.448E23\ T^{-9}$

(600.61 < T < 1200)

$4157.616 + 53.139072\ T - 18.9640637\ T\ln(T) - 2.882943E{-3}\ T^2 + 0.098144E{-6}\ T^3 - 2696755\ T^{-1}$
$+ 805.448E23\ T^{-9}$ *(1200 < T < 2100)*

LIQUID

$-2977.961 + 93.949561\ T - 24.5242231\ T\ln(T) - 3.65895E{-3}\ T^2 - 0.24395E{-6}\ T^3 - 60.19E{-20}\ T^7$

(298.15 < T < 600.61)

$-5677.958 + 146.176046\ T - 32.4913959\ T\ln(T) + 1.54613E{-3}\ T^2$ *(600.61 < T < 1200)*

$9010.753 + 45.071937\,T - 18.9640637\,T\ln(T) - 2.882943E\text{-}3\,T^2 + 0.098144E\text{-}6\,T^3 - 2696755\,T^{-1}$
$(1200 < T < 2100)$

BCT_A5

$-7161.085 + 105.220244\,T - 24.5242231\,T\ln(T) - 3.65895E\text{-}3\,T^2 - 0.24395E\text{-}6\,T^3$
$(298.15 < T < 600.61)$
$-10042.095 + 157.763182\,T - 32.4913959\,T\ln(T) + 1.54613E\text{-}3\,T^2 + 805.448E23\,T^{-9}$
$(600.61 < T < 1200)$
$4646.616 + 56.659072\,T - 18.9640637\,T\ln(T) - 2.882943E\text{-}3\,T^2 + 0.098144E\text{-}6\,T^3 - 2696755\,T^{-1}$
$+ 805.448E23\,T^{-9}$ *$(1200 < T < 2100)$*

RHOMBOHEDRAL_A7

$-7350.085 + 102.700244\,T - 24.5242231\,T\ln(T) - 3.65895E\text{-}3\,T^2 - 0.24395E\text{-}6\,T^3$
$(298.15 < T < 600.61)$
$-10231.095 + 155.243182\,T - 32.4913959\,T\ln(T) + 1.54613E\text{-}3\,T^2 + 805.448E23\,T^{-9}$
$(600.61 < T < 1200)$
$4457.616 + 54.139072\,T - 18.9640637\,T\ln(T) - 2.882943E\text{-}3\,T^2 + 0.098144E\text{-}6\,T^3 - 2696755\,T^{-1}$
$+ 805.448E23\,T^{-9}$ *$(1200 < T < 2100)$*

TETRAGONAL_A6

$-3156.85 + 101.700244\,T - 24.5242231\,T\ln(T) - 3.65895E\text{-}3\,T^2 - 0.24395E\text{-}6\,T^3$ *$(298.15 < T < 600.61)$*
$-6037.86 + 154.243182\,T - 32.4913959\,T\ln(T) + 1.54613E\text{-}3\,T^2 + 805.448E23\,T^{-9}$
$(600.61 < T < 1200)$
$8650.851 + 53.139072\,T - 18.9640637\,T\ln(T) - 2.882943E\text{-}3\,T^2 + 0.098144E\text{-}6\,T^3 - 2696755\,T^{-1}$
$+ 805.448E23\,T^{-9}$ *$(1200 < T < 2100)$*

TET_ALPHA1

$-5746.785 + 99.640044\,T - 24.5242231\,T\ln(T) - 3.65895E\text{-}3\,T^2 - 0.24395E\text{-}6\,T^3$ *$(298.15 < T < 600.61)$*
$-8627.795 + 152.182982\,T - 32.4913959\,T\ln(T) + 1.54613E\text{-}3\,T^2 + 805.448E23\,T^{-9}$
$(600.61 < T < 1200)$
$6060.916 + 51.078872\,T - 18.9640637\,T\ln(T) - 2.882943E\text{-}3\,T^2 + 0.098144E\text{-}6\,T^3 - 2696755\,T^{-1}$
$+ 805.448E23\,T^{-9}$ *$(1200 < T < 2100)$*

BCC_A2

$-5250.085 + 100.600244\,T - 24.5242231\,T\ln(T) - 3.65895E\text{-}3\,T^2 - 0.24395E\text{-}6\,T^3$
$(298.15 < T < 600.61)$
$-8131.095 + 153.143182\,T - 32.4913959\,T\ln(T) + 1.54613E\text{-}3\,T^2 + 805.448E23\,T^{-9}$
$(600.61 < T < 1200)$
$6557.616 + 52.039072\,T - 18.9640637\,T\ln(T) - 2.882943E\text{-}3\,T^2 + 0.098144E\text{-}6\,T^3 - 2696755\,T^{-1}$
$+ 805.448E23\,T^{-9}$ *$(1200 < T < 2100)$*

HCP_A3

$-7350.085 + 102.700244\ T - 24.5242231\ T \ln(T) - 3.65895E{-3}\ T^2 - 0.24395E{-6}\ T^3$ *(298.15 < T < 600.61)*

$-10231.095 + 155.243182\ T - 32.4913959\ T \ln(T) + 1.54613E{-3}\ T^2 + 805.448E23\ T^{-9}$ *(600.61 < T < 1200)*

$4457.616 + 54.139072\ T - 18.9640637\ T \ln(T) - 2.882943E{-3}\ T^2 + 0.098144E{-6}\ T^3 - 2696755\ T^{-1} + 805.448E23\ T^{-9}$ *(1200 < T < 2100)*

RHOMBO_A10

$-7640.085 + 101.700244\ T - 24.5242231\ T \ln(T) - 3.65895E{-3}\ T^2 - 0.24395E{-6}\ T^3$ *(298.15 < T < 600.61)*

$-10521.095 + 154.243182\ T - 32.4913959\ T \ln(T) + 1.54613E{-3}\ T^2 + 805.448E23\ T^{-9}$ *(600.61 < T < 1200)*

$4167.616 + 53.139072\ T - 18.9640637\ T \ln(T) - 2.882943E{-3}\ T^2 + 0.098144E{-6}\ T^3 - 2696755\ T^{-1} + 805.448E23\ T^{-9}$ *(1200 < T < 2100)*

Data relative to FCC_A1

LIQUID

$4672.124 - 7.750683\ T - 60.19E{-20}\ T^7$ *(298.15 < T < 600.61)*

$4853.137 - 8.067136\ T - 805.448E23\ T^{-9}$ *(600.61 < T < 2100)*

BCT_A5

$489 + 3.52\ T$ *(298.15 < T < 2100)*

RHOMBOHEDRAL_A7

$300 + 1\ T$ *(298.15 < T < 2100)*

TETRAGONAL_A6

4493.235 *(298.15 < T < 2100)*

TET_ALPHA1

$1903.3 - 2.0602\ T$ *(298.15 < T < 2100)*

BCC_A2

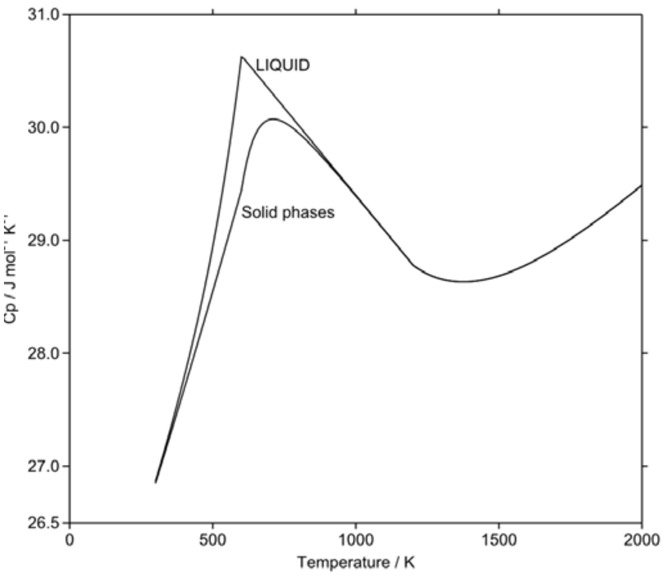
$2400 - 1.1\ T$ *(298.15 < T < 2100)*

HCP_A3

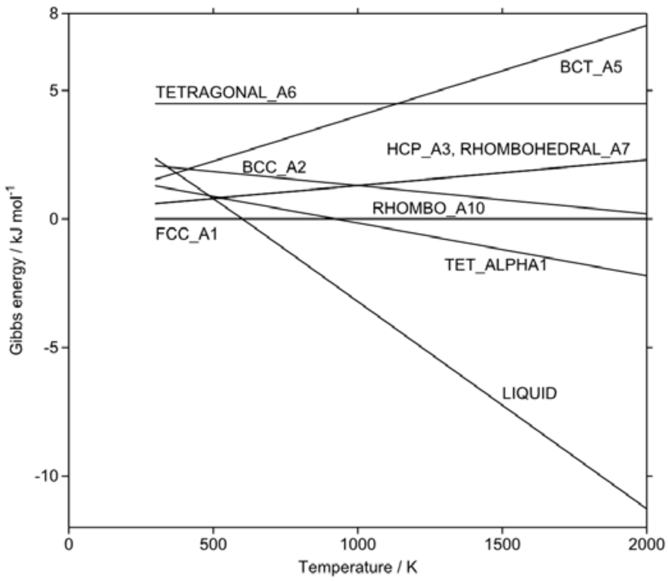
300 + 1 T *(298.15 < T < 2100)*

RHOMBO_A10

10 *(298.15 < T < 2100)*



Heat capacity of Pb



Gibbs energy of phases of Pb relative to FCC_A1

Pd

Source of data: *A T Dinsdale, Unpublished work [FCC_A1, LIQUID]*
Saunders et al. [BCC_A2, HCP_A3]
J. Vrestal, J. Pinkas, A. Watson, A. Scott, J. Houserova, A. Kroupa, CALPHAD 2006, 30(1) 14-17 [RHOMBOHEDRAL_A7]

FCC_A1

$-10204.027 + 176.076315\ T - 32.211\ T \ln(T) + 7.120975E\text{-}3\ T^2 - 1.919875E\text{-}6\ T^3 + 168687\ T^{-1}$ *(298.15 < T < 900)*

$917.062 + 49.659892\ T - 13.5708\ T \ln(T) - 7.17522E\text{-}3\ T^2 + 0.191115E\text{-}6\ T^3 - 1112465\ T^{-1}$ *(900 < T < 1828)*

$-67161.018 + 370.102147\ T - 54.2067086\ T \ln(T) + 2.091396E\text{-}3\ T^2 - 0.062811E\text{-}6\ T^3 + 18683526\ T^{-1}$ *(1828 < T < 4000)*

LIQUID

$1302.731 + 170.964153\ T - 32.211\ T \ln(T) + 7.120975E\text{-}3\ T^2 - 1.919875E\text{-}6\ T^3 + 168687\ T^{-1}$ *(298.15 < T < 600)*

$23405.778 - 116.918419\,T + 10.8922031\,T\ln(T) - 27.266568E{-3}\,T^2 + 2.430675E{-6}\,T^3 - 1853674\,T^{-1}$

(600 < T < 1828)

$-12373.637 + 251.416903\,T - 41.17\,T\ln(T)$ *(1828 < T < 4000)*

BCC_A2

$295.973 + 174.276315\,T - 32.211\,T\ln(T) + 7.120975E{-3}\,T^2 - 1.919875E{-6}\,T^3 + 168687\,T^{-1}$

(298.15 < T < 900)

$11417.062 + 47.859892\,T - 13.5708\,T\ln(T) - 7.17522E{-3}\,T^2 + 0.191115E{-6}\,T^3 - 1112465\,T^{-1}$

(900 < T < 1828)

$-56661.018 + 368.302147\,T - 54.2067086\,T\ln(T) + 2.091396E{-3}\,T^2 - 0.062811E{-6}\,T^3 + 18683526\,T^{-1}$

(1828 < T < 4000)

HCP_A3

$-8204.027 + 176.176315\,T - 32.211\,T\ln(T) + 7.120975E{-3}\,T^2 - 1.919875E{-6}\,T^3 + 168687\,T^{-1}$

(298.15 < T < 900)

$2917.062 + 49.759892\,T - 13.5708\,T\ln(T) - 7.17522E{-3}\,T^2 + 0.191115E{-6}\,T^3 - 1112465\,T^{-1}$

(900 < T < 1828)

$-65161.018 + 370.202147\,T - 54.2067086\,T\ln(T) + 2.091396E{-3}\,T^2 - 0.062811E{-6}\,T^3 + 18683526\,T^{-1}$

(1828 < T < 4000)

RHOMBOHEDRAL_A7

$-6204.027 + 176.076315\,T - 32.211\,T\ln(T) + 7.120975E{-3}\,T^2 - 1.919875E{-6}\,T^3 + 168687\,T^{-1}$

(298.15 < T < 900)

$4917.062 + 49.659892\,T - 13.5708\,T\ln(T) - 7.17522E{-3}\,T^2 + 0.191115E{-6}\,T^3 - 1112465\,T^{-1}$

(900 < T < 1828)

$-63161.018 + 370.102147\,T - 54.2067086\,T\ln(T) + 2.091396E{-3}\,T^2 - 0.062811E{-6}\,T^3 + 18683526\,T^{-1}$

(1828 < T < 4000)

Data relative to FCC_A1

LIQUID

$11506.758 - 5.112162\,T$ *(298.15 < T < 600)*

$33609.805 - 292.994734\,T + 43.1032031\,T\ln(T) - 34.387543E{-3}\,T^2 + 4.35055E{-6}\,T^3 - 2022361\,T^{-1}$

(600 < T < 900)

$22488.716 - 166.578311\,T + 24.4630031\,T\ln(T) - 20.091348E{-3}\,T^2 + 2.23956E{-6}\,T^3 - 741209\,T^{-1}$

(900 < T < 1828)

$54787.381 - 118.685244\,T + 13.0367086\,T\ln(T) - 2.091396E{-3}\,T^2 + 0.062811E{-6}\,T^3 - 18683526\,T^{-1}$

(1828 < T < 4000)

BCC_A2

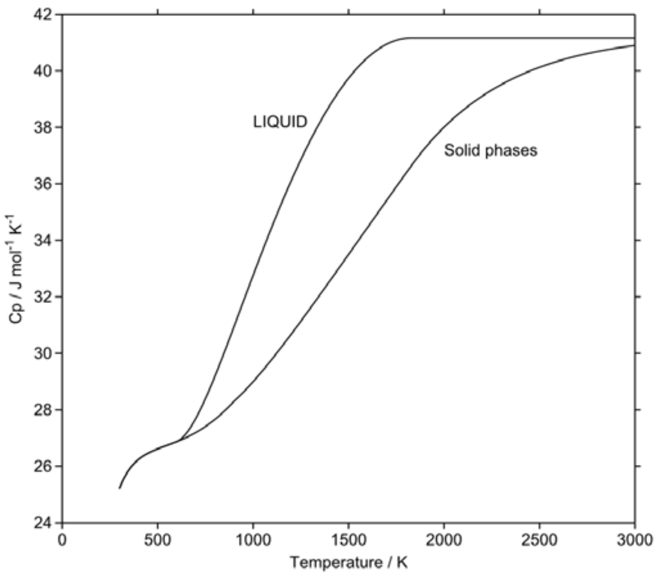
$10500 - 1.8\,T$ *(298.15 < T < 4000)*

HCP_A3

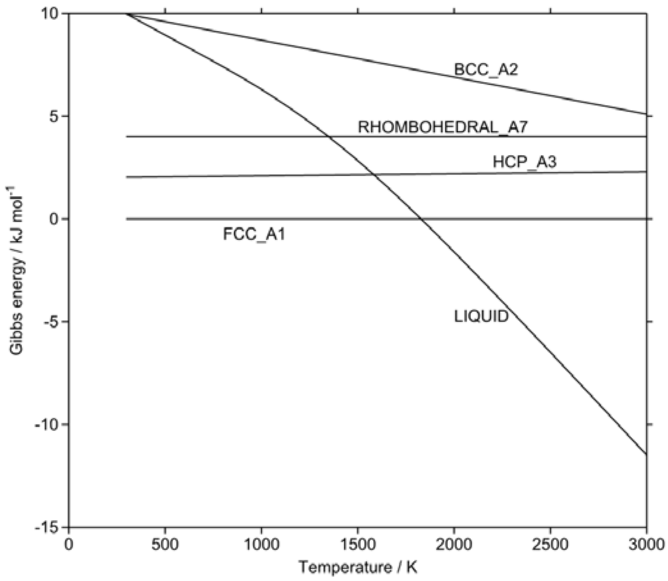
2000 + 0.1 T *(298.15 < T < 4000)*

RHOMBOHEDRAL_A7

4000 *(298.15 < T < 4000)*



Heat capacity of Pd



Gibbs energy of phases of Pd relative to FCC_A1

Pr

Source of data: *Hultgren*

DHCP

$-18803.379 + 356.587384\ T - 68.9176\ T\ \ln(T) + 72.929E\text{-}3\ T^2 - 25.184333E\text{-}6\ T^3 + 507385\ T^{-1}$ *(298.15 < T < 500)*

$-7246.848 + 82.427384\ T - 22.8909\ T\ \ln(T) - 4.97126E\text{-}3\ T^2 - 1.22951E\text{-}6\ T^3$ *(500 < T < 800)*

$95411.023 - 1073.551114\ T + 146.764\ T\ \ln(T) - 128.8205E\text{-}3\ T^2 + 15.592233E\text{-}6\ T^3 - 11588800\ T^{-1}$ *(800 < T < 1068)*

$-481663.131 + 4234.333112\ T - 606.1203107\ T\ \ln(T) + 305.181506E\text{-}3\ T^2 - 30.994702E\text{-}6\ T^3 + 70926840\ T^{-1}$ *(1068 < T < 1204)*

$-20014.678 + 227.685155\ T - 42.9697\ T\ \ln(T)$ *(1204 < T < 3800)*

BCC_A2

$-2863.651 + 28.274853\ T - 13.7470527\ T\ \ln(T) - 22.84377E\text{-}3\ T^2 + 3.542468E\text{-}6\ T^3 - 87486\ T^{-1}$ *(298.15 < T < 1068)*

$-11985.919 + 188.657121\ T - 38.451\ T\ \ln(T)$ *(1068 < T < 1204)*

$953.224 + 100.826281\ T - 26.6824313\ T\ln(T) - 4.106833E\text{-}3\ T^2 + 0.176214E\text{-}6\ T^3 - 2473024\ T^{-1}$
(1204 < T < 3800)

LIQUID

$3848.961 - 29.099465\ T - 4.7344931\ T\ln(T) - 35.119723E\text{-}3\ T^2 + 5.427467E\text{-}6\ T^3 - 207406\ T^{-1}$
(298.15 < T < 1068)
$-10539.574 + 219.508805\ T - 42.9697\ T\ln(T)$ *(1068 < T < 3800)*

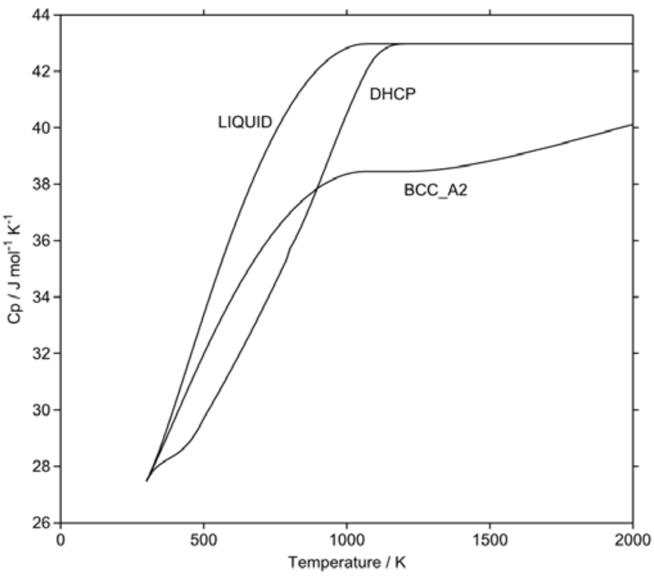
Data relative to DHCP

BCC_A2

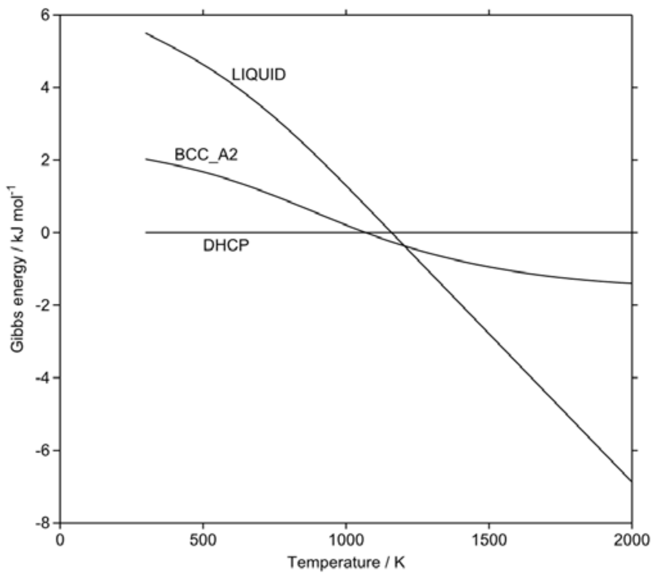
$15939.728 - 328.312531\ T + 55.1705473\ T\ln(T) - 95.77277E\text{-}3\ T^2 + 28.726801E\text{-}6\ T^3 - 594871\ T^{-1}$
(298.15 < T < 500)
$4383.197 - 54.152531\ T + 9.1438473\ T\ln(T) - 17.87251E\text{-}3\ T^2 + 4.771978E\text{-}6\ T^3 - 87486\ T^{-1}$
(500 < T < 800)
$-98274.674 + 1101.825967\ T - 160.5110527\ T\ln(T) + 105.97673E\text{-}3\ T^2 - 12.049765E\text{-}6\ T^3$
$+ 11501314\ T^{-1}$ *(800 < T < 1068)*
$469677.212 - 4045.675991\ T + 567.6693107\ T\ln(T) - 305.181506E\text{-}3\ T^2 + 30.994702E\text{-}6\ T^3$
$- 70926840\ T^{-1}$ *(1068 < T < 1204)*
$20967.902 - 126.858874\ T + 16.2872687\ T\ln(T) - 4.106833E\text{-}3\ T^2 + 0.176214E\text{-}6\ T^3 - 2473024\ T^{-1}$
(1204 < T < 3800)

LIQUID

$22652.34 - 385.686849\ T + 64.1831069\ T\ln(T) - 108.048723E\text{-}3\ T^2 + 30.6118E\text{-}6\ T^3 - 714791\ T^{-1}$
(298.15 < T < 500)
$11095.809 - 111.526849\ T + 18.1564069\ T\ln(T) - 30.148463E\text{-}3\ T^2 + 6.656977E\text{-}6\ T^3 - 207406\ T^{-1}$
(500 < T < 800)
$-91562.062 + 1044.451649\ T - 151.4984931\ T\ln(T) + 93.700777E\text{-}3\ T^2 - 10.164766E\text{-}6\ T^3$
$+ 11381394\ T^{-1}$ *(800 < T < 1068)*
$471123.557 - 4014.824307\ T + 563.1506107\ T\ln(T) - 305.181506E\text{-}3\ T^2 + 30.994702E\text{-}6\ T^3$
$- 70926840\ T^{-1}$ *(1068 < T < 1204)*
$9475.104 - 8.17635\ T$ *(1204 < T < 3800)*



Heat capacity of Pr



Gibbs energy of phases of Pr relative to DHCP

Pt

Source of data: *A T Dinsdale, Unpublished work, [FCC_A1, LIQUID]*
Saunders et al. [BCC_A2, HCP_A3]

FCC_A1

$-7595.631 + 124.388275\ T - 24.5526\ T \ln(T) - 2.48297E\text{-}3\ T^2 - 0.020138E\text{-}6\ T^3 + 7974\ T^{-1}$
(298.15 < T < 1300)

$-9253.174 + 161.529615\ T - 30.2527\ T \ln(T) + 2.321665E\text{-}3\ T^2 - 0.656946E\text{-}6\ T^3 - 272106\ T^{-1}$
(1300 < T < 2041.5)

$-222048.216 + 1019.358919\ T - 136.192996\ T \ln(T) + 20.454938E\text{-}3\ T^2 - 0.759259E\text{-}6\ T^3 + 71539020\ T^{-1}$
(2041.5 < T < 4000)

LIQUID

$12518.385 + 115.113092\ T - 24.5526\ T \ln(T) - 2.48297E\text{-}3\ T^2 - 0.020138E\text{-}6\ T^3 + 7974\ T^{-1}$
(298.15 < T < 600)

$19023.491 + 32.94182\ T - 12.3403769\ T \ln(T) - 11.551507E\text{-}3\ T^2 + 0.931516E\text{-}6\ T^3 - 601426\ T^{-1}$
(600 < T < 2041.5)

$1404.468 + 205.858962\ T - 36.5\ T \ln(T)$ *(2041.5 < T < 4000)*

BCC_A2

$7404.369 + 121.988275\ T - 24.5526\ T \ln(T) - 2.48297E\text{-}3\ T^2 - 0.020138E\text{-}6\ T^3 + 7974\ T^{-1}$
(298.15 < T < 1300)

$5746.826 + 159.129615\ T - 30.2527\ T \ln(T) + 2.321665E\text{-}3\ T^2 - 0.656946E\text{-}6\ T^3 - 272106\ T^{-1}$
(1300 < T < 2041.5)

$-207048.216 + 1016.958919\,T - 136.192996\,T\ln(T) + 20.454938E{-3}\,T^2 - 0.759259E{-6}\,T^3 + 71539020\,T^{-1}$ *(2041.5 < T < 4000)*

HCP_A3

$-5095.631 + 124.488275\,T - 24.5526\,T\ln(T) - 2.48297E{-3}\,T^2 - 0.020138E{-6}\,T^3 + 7974\,T^{-1}$ *(298.15 < T < 1300)*

$-6753.174 + 161.629615\,T - 30.2527\,T\ln(T) + 2.321665E{-3}\,T^2 - 0.656946E{-6}\,T^3 - 272106\,T^{-1}$ *(1300 < T < 2041.5)*

$-219548.216 + 1019.458919\,T - 136.192996\,T\ln(T) + 20.454938E{-3}\,T^2 - 0.759259E{-6}\,T^3 + 71539020\,T^{-1}$ *(2041.5 < T < 4000)*

Data relative to FCC_A1

LIQUID

$20114.016 - 9.275183\,T$ *(298.15 < T < 600)*

$26619.122 - 91.446455\,T + 12.2122231\,T\ln(T) - 9.068537E{-3}\,T^2 + 0.951654E{-6}\,T^3 - 609400\,T^{-1}$ *(600 < T < 1300)*

$28276.665 - 128.587795\,T + 17.9123231\,T\ln(T) - 13.873172E{-3}\,T^2 + 1.588462E{-6}\,T^3 - 329320\,T^{-1}$ *(1300 < T < 2041.5)*

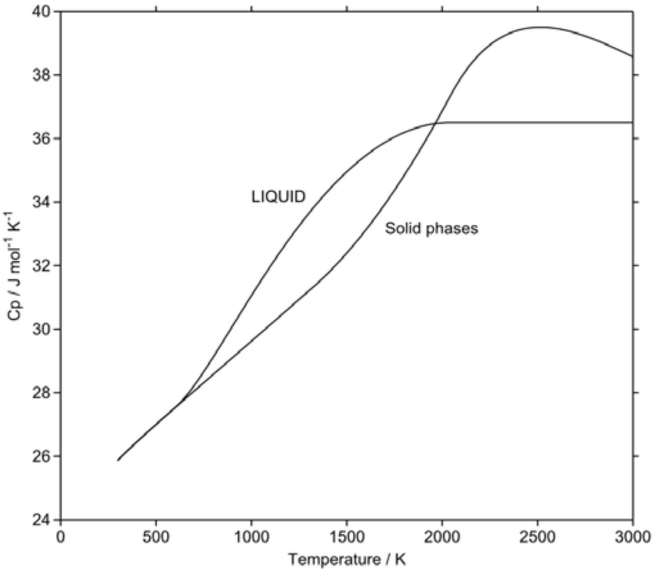
$223452.684 - 813.499957\,T + 99.692996\,T\ln(T) - 20.454938E{-3}\,T^2 + 0.759259E{-6}\,T^3 - 71539020\,T^{-1}$ *(2041.5 < T < 4000)*

BCC_A2

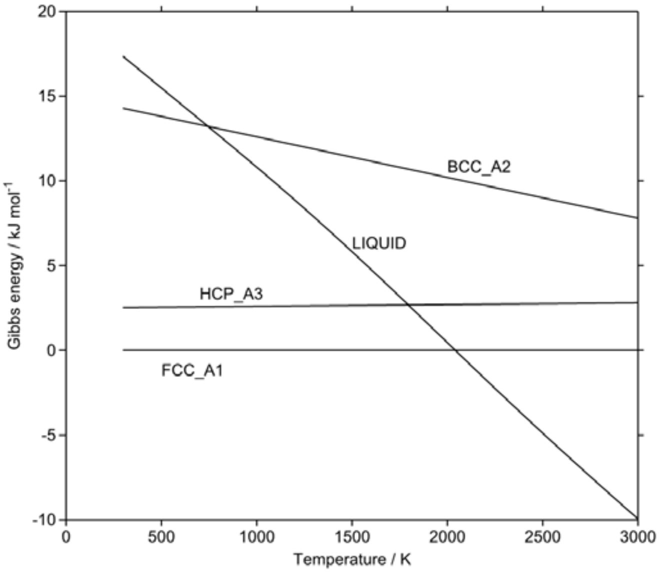
$15000 - 2.4\,T$ *(298.15 < T < 4000)*

HCP_A3

$2500 + 0.1\,T$ *(298.15 < T < 4000)*



Heat capacity of Pt



Gibbs energy of phases of Pt relative to FCC_A1

Pu

Source of data: *M H Rand and A T Dinsdale, Unpublished work*

ALPHA_PU

$-7396.309 + 80.301382\ T - 18.1258\ T\ln(T) - 22.41E\text{-}3\ T^2$ *(298.15 < T < 400)*
$-16605.962 + 236.786603\ T - 42.4187\ T\ln(T) - 1.34493E\text{-}3\ T^2 + 0.263443E\text{-}6\ T^3 + 579325\ T^{-1}$
(400 < T < 944)
$-14462.156 + 232.961553\ T - 42.248\ T\ln(T)$ *(944 < T < 3000)*

BETA_PU

$-4873.654 + 123.249151\ T - 27.416\ T\ln(T) - 6.53E\text{-}3\ T^2$ *(298.15 < T < 679.5)*
$2435.094 + 43.566585\ T - 15.7351\ T\ln(T) - 15.4772E\text{-}3\ T^2 + 1.524942E\text{-}6\ T^3 - 864940\ T^{-1}$
(679.5 < T < 1464)
$-13959.062 + 228.221615\ T - 42.248\ T\ln(T)$ *(1464 < T < 3000)*

GAMMA_PU

$-16766.303 + 419.402655\ T - 77.5802\ T\ln(T) + 81.6415E\text{-}3\ T^2 - 28.103833E\text{-}6\ T^3 + 574825\ T^{-1}$
(298.15 < T < 487.9)
$-2942.77 + 88.325069\ T - 22.0233\ T\ln(T) - 11.4795E\text{-}3\ T^2$ *(487.9 < T < 593.9)*
$-9336.967 + 160.314641\ T - 32.3405\ T\ln(T) - 7.0383E\text{-}3\ T^2 + 0.692887E\text{-}6\ T^3 + 630600\ T^{-1}$
(593.9 < T < 1179)
$-12435.75 + 226.131617\ T - 42.248\ T\ln(T)$ *(1179 < T < 3000)*

FCC_A1

$-3920.781 + 127.586536\, T - 28.4781\, T \ln(T) - 5.4035E{-3}\, T^2$ *(298.15 < T < 990)*
$3528.208 + 41.52572\, T - 15.7351\, T \ln(T) - 15.4772E{-3}\, T^2 + 1.524942E{-6}\, T^3 - 864940\, T^{-1}$
(990 < T < 1464)
$-12865.948 + 226.18075\, T - 42.248\, T \ln(T)$ *(1464 < T < 3000)*

TETRAGONAL_A6

$-496.178 + 54.586547\, T - 16.43\, T \ln(T) - 24.006E{-3}\, T^2 + 5.166667E{-6}\, T^3 - 158470\, T^{-1}$
(298.15 < T < 736)
$-6122.307 + 173.35008\, T - 35.56\, T \ln(T)$ *(736 < T < 757)*
$3982.078 + 63.890352\, T - 19.756\, T \ln(T) - 9.37295E{-3}\, T^2 + 0.659882E{-6}\, T^3 - 1112565\, T^{-1}$
(757 < T < 2157)
$-15200.539 + 228.05641\, T - 42.248\, T \ln(T)$ *(2157 < T < 3000)*

BCC_A2

$-1358.984 + 116.603882\, T - 27.094\, T \ln(T) - 9.105E{-3}\, T^2 + 2.061667E{-6}\, T^3 + 20863\, T^{-1}$
(298.15 < T < 745)
$-2890.817 + 156.878957\, T - 33.72\, T \ln(T)$ *(745 < T < 956)*
$29313.619 - 132.788248\, T + 6.921\, T \ln(T) - 20.23305E{-3}\, T^2 + 1.426922E{-6}\, T^3 - 4469245\, T^{-1}$
(956 < T < 2071)
$-15400.585 + 227.421855\, T - 42.248\, T \ln(T)$ *(2071 < T < 3000)*

LIQUID

$-788.209 + 67.788082\, T - 18.1258\, T \ln(T) - 22.41E{-3}\, T^2$ *(298.15 < T < 400)*
$-9997.862 + 224.273303\, T - 42.4187\, T \ln(T) - 1.34493E{-3}\, T^2 + 0.263443E{-6}\, T^3 + 579325\, T^{-1}$
(400 < T < 944)
$-7854.056 + 220.448253\, T - 42.248\, T \ln(T)$ *(944 < T < 3000)*

Data relative to ALPHA_PU

BETA_PU

$2522.655 + 42.947769\, T - 9.2902\, T \ln(T) + 15.88E{-3}\, T^2$ *(298.15 < T < 400)*
$11732.308 - 113.537452\, T + 15.0027\, T \ln(T) - 5.18507E{-3}\, T^2 - 0.263443E{-6}\, T^3 - 579325\, T^{-1}$
(400 < T < 679.5)
$19041.056 - 193.220018\, T + 26.6836\, T \ln(T) - 14.13227E{-3}\, T^2 + 1.261499E{-6}\, T^3 - 1444265\, T^{-1}$
(679.5 < T < 944)
$16897.25 - 189.394968\, T + 26.5129\, T \ln(T) - 15.4772E{-3}\, T^2 + 1.524942E{-6}\, T^3 - 864940\, T^{-1}$
(944 < T < 1464)
$503.094 - 4.739938\, T$ *(1464 < T < 3000)*

GAMMA_PU

$-9369.994 + 339.101273\ T - 59.4544\ T\ln(T) + 104.0515E{-3}\ T^2 - 28.103833E{-6}\ T^3 + 574825\ T^{-1}$ *(298.15 < T < 400)*

$-160.341 + 182.616052\ T - 35.1615\ T\ln(T) + 82.98643E{-3}\ T^2 - 28.367276E{-6}\ T^3 - 4500\ T^{-1}$ *(400 < T < 487.9)*

$13663.192 - 148.461534\ T + 20.3954\ T\ln(T) - 10.13457E{-3}\ T^2 - 0.263443E{-6}\ T^3 - 579325\ T^{-1}$ *(487.9 < T < 593.9)*

$7268.995 - 76.471962\ T + 10.0782\ T\ln(T) - 5.69337E{-3}\ T^2 + 0.429444E{-6}\ T^3 + 51275\ T^{-1}$ *(593.9 < T < 944)*

$5125.189 - 72.646912\ T + 9.9075\ T\ln(T) - 7.0383E{-3}\ T^2 + 0.692887E{-6}\ T^3 + 630600\ T^{-1}$ *(944 < T < 1179)*

$2026.406 - 6.829936\ T$ *(1179 < T < 3000)*

FCC_A1

$3475.528 + 47.285154\ T - 10.3523\ T\ln(T) + 17.0065E{-3}\ T^2$ *(298.15 < T < 400)*

$12685.181 - 109.200067\ T + 13.9406\ T\ln(T) - 4.05857E{-3}\ T^2 - 0.263443E{-6}\ T^3 - 579325\ T^{-1}$ *(400 < T < 944)*

$10541.375 - 105.375017\ T + 13.7699\ T\ln(T) - 5.4035E{-3}\ T^2$ *(944 < T < 990)*

$17990.364 - 191.435833\ T + 26.5129\ T\ln(T) - 15.4772E{-3}\ T^2 + 1.524942E{-6}\ T^3 - 864940\ T^{-1}$ *(990 < T < 1464)*

$1596.208 - 6.780803\ T$ *(1464 < T < 3000)*

TETRAGONAL_A6

$6900.131 - 25.714835\ T + 1.6958\ T\ln(T) - 1.596E{-3}\ T^2 + 5.166667E{-6}\ T^3 - 158470\ T^{-1}$ *(298.15 < T < 400)*

$16109.784 - 182.200056\ T + 25.9887\ T\ln(T) - 22.66107E{-3}\ T^2 + 4.903224E{-6}\ T^3 - 737795\ T^{-1}$ *(400 < T < 736)*

$10483.655 - 63.436523\ T + 6.8587\ T\ln(T) + 1.34493E{-3}\ T^2 - 0.263443E{-6}\ T^3 - 579325\ T^{-1}$ *(736 < T < 757)*

$20588.04 - 172.896251\ T + 22.6627\ T\ln(T) - 8.02802E{-3}\ T^2 + 0.396439E{-6}\ T^3 - 1691890\ T^{-1}$ *(757 < T < 944)*

$18444.234 - 169.071201\ T + 22.492\ T\ln(T) - 9.37295E{-3}\ T^2 + 0.659882E{-6}\ T^3 - 1112565\ T^{-1}$ *(944 < T < 2157)*

$-738.383 - 4.905143\ T$ *(2157 < T < 3000)*

BCC_A2

$6037.325 + 36.3025\ T - 8.9682\ T\ln(T) + 13.305E{-3}\ T^2 + 2.061667E{-6}\ T^3 + 20863\ T^{-1}$ *(298.15 < T < 400)*

$15246.978 - 120.182721\ T + 15.3247\ T\ln(T) - 7.76007E{-3}\ T^2 + 1.798224E{-6}\ T^3 - 558462\ T^{-1}$ *(400 < T < 745)*

$13715.145 - 79.907646\ T + 8.6987\ T\ln(T) + 1.34493E{-3}\ T^2 - 0.263443E{-6}\ T^3 - 579325\ T^{-1}$ *(745 < T < 944)*

$11571.339 - 76.082596\ T + 8.528\ T\ln(T)$ *(944 < T < 956)*

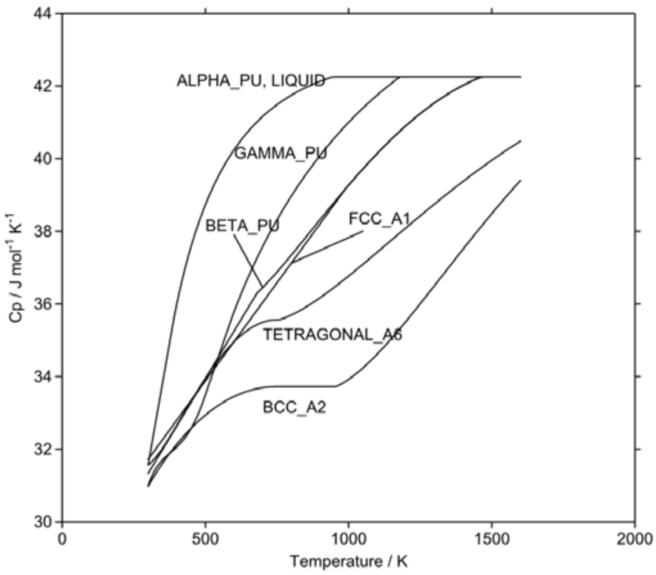
$43775.775 - 365.749801\ T + 49.169\ T\ln(T) - 20.23305E{-3}\ T^{2} + 1.426922E{-6}\ T^{3} - 4469245\ T^{-1}$

(956 < T < 2071)

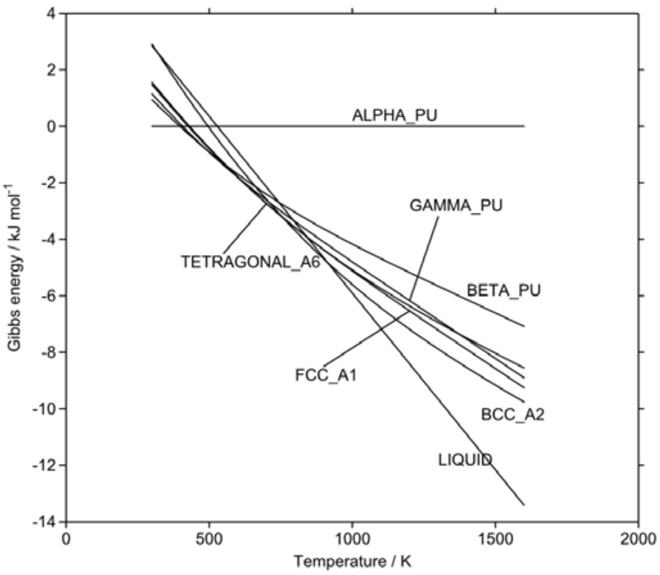
$-938.429 - 5.539698\ T$ *(2071 < T < 3000)*

LIQUID

$6608.1 - 12.5133\ T$ *(298.15 < T < 3000)*



Heat capacity of Pu



Gibbs energy of phases of Pu relative to ALPHA_PU

Rb

Source of data: *TPIS [BCC_A2, LIQUID]*
Saunders et al. [HCP_A3, FCC_A1]

BCC_A2

$-21669.733 + 583.580988\ T - 115.2825888\ T\ln(T) + 262.77612E{-3}\ T^{2} - 152.236932E{-6}\ T^{3} + 385754\ T^{-1}$

(200 < T < 312.46)

$-7823.397 + 117.050578\ T - 29.1775424\ T\ln(T) + 0.412369E{-3}\ T^{2} - 0.46822E{-6}\ T^{3} - 126310\ T^{-1}$
$- 555.029E20\ T^{-9}$ *(312.46 < T < 900)*

$-39488.142 + 450.974149\ T - 77.7006456\ T\ln(T) + 33.795632E{-3}\ T^{2} - 4.829082E{-6}\ T^{3} + 3778006\ T^{-1}$
$- 555.029E20\ T^{-9}$ *(900 < T < 1600)*

$-159742.511 + 1287.789466\ T - 191.2627736\ T\ln(T) + 81.61687E{-3}\ T^{2} - 8.61653E{-6}\ T^{3} + 27738456\ T^{-1}$
$- 555.029E20\ T^{-9}$ *(1600 < T < 2100)*

LIQUID

$-19452.181 + 576.470502\ T - 115.2825888\ T \ln(T) + 262.77612E\text{-}3\ T^2 - 152.236932E\text{-}6\ T^3 + 385754\ T^{-1} + 144.078E\text{-}19\ T^7$ *(200 < T < 312.46)*

$-5650.532 + 110.090262\ T - 29.1775424\ T \ln(T) + 0.412369E\text{-}3\ T^2 - 0.46822E\text{-}6\ T^3 - 126310\ T^{-1}$ *(312.46 < T < 900)*

$-37315.276 + 444.013833\ T - 77.7006456\ T \ln(T) + 33.795632E\text{-}3\ T^2 - 4.829082E\text{-}6\ T^3 + 3778006\ T^{-1}$ *(900 < T < 1600)*

$-157569.646 + 1280.829151\ T - 191.2627736\ T \ln(T) + 81.61687E\text{-}3\ T^2 - 8.61653E\text{-}6\ T^3 + 27738456\ T^{-1}$ *(1600 < T < 2100)*

FCC_A1

$-21469.733 + 584.880988\ T - 115.2825888\ T \ln(T) + 262.77612E\text{-}3\ T^2 - 152.236932E\text{-}6\ T^3 + 385754\ T^{-1}$ *(200 < T < 312.46)*

$-7623.397 + 118.350578\ T - 29.1775424\ T \ln(T) + 0.412369E\text{-}3\ T^2 - 0.46822E\text{-}6\ T^3 - 126310\ T^{-1} - 555.029E20\ T^{-9}$ *(312.46 < T < 900)*

$-39288.142 + 452.274149\ T - 77.7006456\ T \ln(T) + 33.795632E\text{-}3\ T^2 - 4.829082E\text{-}6\ T^3 + 3778006\ T^{-1} - 555.029E20\ T^{-9}$ *(900 < T < 1600)*

$-159542.511 + 1289.089466\ T - 191.2627736\ T \ln(T) + 81.61687E\text{-}3\ T^2 - 8.61653E\text{-}6\ T^3 + 27738456\ T^{-1} - 555.029E20\ T^{-9}$ *(1600 < T < 2100)*

HCP_A3

$-21469.733 + 585.580988\ T - 115.2825888\ T \ln(T) + 262.77612E\text{-}3\ T^2 - 152.236932E\text{-}6\ T^3 + 385754\ T^{-1}$ *(200 < T < 312.46)*

$-7623.397 + 119.050578\ T - 29.1775424\ T \ln(T) + 0.412369E\text{-}3\ T^2 - 0.46822E\text{-}6\ T^3 - 126310\ T^{-1} - 555.029E20\ T^{-9}$ *(312.46 < T < 900)*

$-39288.142 + 452.974149\ T - 77.7006456\ T \ln(T) + 33.795632E\text{-}3\ T^2 - 4.829082E\text{-}6\ T^3 + 3778006\ T^{-1} - 555.029E20\ T^{-9}$ *(900 < T < 1600)*

$-159542.511 + 1289.789466\ T - 191.2627736\ T \ln(T) + 81.61687E\text{-}3\ T^2 - 8.61653E\text{-}6\ T^3 + 27738456\ T^{-1} - 555.029E20\ T^{-9}$ *(1600 < T < 2100)*

Data relative to BCC_A2

LIQUID

$2217.552 - 7.110486\ T + 144.078E\text{-}19\ T^7$ *(200 < T < 312.46)*

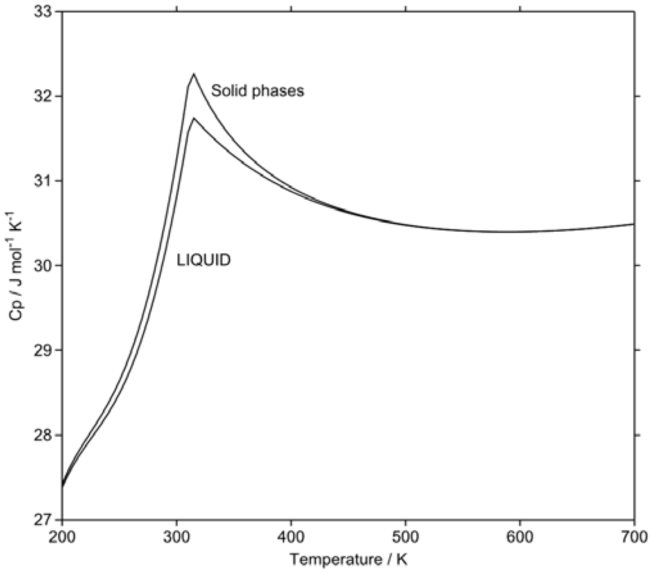
$2172.865 - 6.960316\ T + 555.029E20\ T^{-9}$ *(312.46 < T < 2100)*

FCC_A1

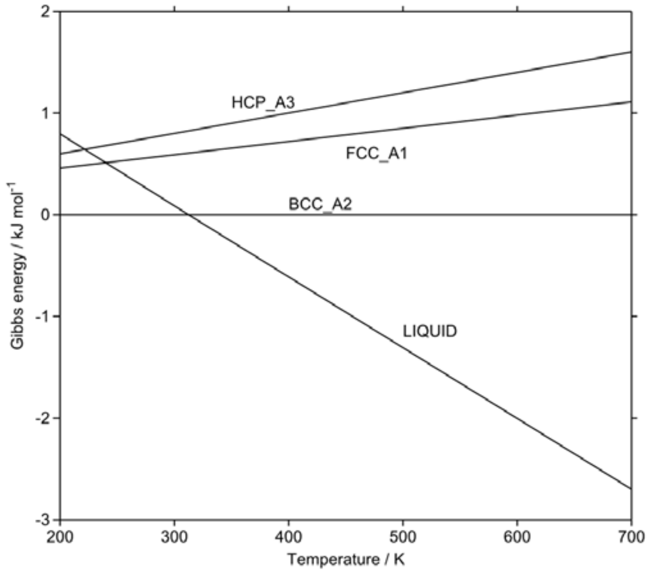
$200 + 1.3\ T$ *(200 < T < 2100)*

HCP_A3

$200 + 2\ T$ *(200 < T < 2100)*



Heat capacity of Rb



Gibbs energy of phases of Rb relative to BCC_A2

Re

Source of data: *J Arblaster, CALPHAD, 1996, 20(3), 343-352 [HCP_A3, LIQUID]*
A T Dinsdale, Unpublished work [BCC_A2, FCC_A1]

HCP_A3

$-7695.279 + 128.421589\ T - 24.348\ T \ln(T) - 2.53505E\text{-}3\ T^2 + 0.192818E\text{-}6\ T^3 + 32915\ T^{-1}$ *(298.15 < T < 1200)*

$-15775.998 + 194.667426\ T - 33.586\ T \ln(T) + 2.24565E\text{-}3\ T^2 - 0.281835E\text{-}6\ T^3 + 1376270\ T^{-1}$ *(1200 < T < 2400)*

$-70882.739 + 462.110749\ T - 67.956\ T \ln(T) + 11.84945E\text{-}3\ T^2 - 0.788955E\text{-}6\ T^3 + 18075200\ T^{-1}$ *(2400 < T < 3458)*

$346325.888 - 1211.371859\ T + 140.8316548\ T \ln(T) - 33.764567E\text{-}3\ T^2 + 1.053726E\text{-}6\ T^3 - 134548866\ T^{-1}$ *(3458 < T < 5000)*

$-78564.296 + 346.997842\ T - 49.519\ T \ln(T)$ *(5000 < T < 6000)*

LIQUID

$16125.604 + 122.076209\ T - 24.348\ T \ln(T) - 2.53505E\text{-}3\ T^2 + 0.192818E\text{-}6\ T^3 + 32915\ T^{-1}$ *(298.15 < T < 1200)*

$8044.885 + 188.322047\ T - 33.586\ T \ln(T) + 2.24565E\text{-}3\ T^2 - 0.281835E\text{-}6\ T^3 + 1376270\ T^{-1}$ *(1200 < T < 2000)*

$568842.665 - 2527.838455\ T + 314.1788975\ T \ln(T) - 89.39817E\text{-}3\ T^2 + 3.92854E\text{-}6\ T^3 - 163100987\ T^{-1}$ *(2000 < T < 3458)*

$-39044.888 + 335.723691\ T - 49.519\ T \ln(T)$ *(3458 < T < 6000)*

BCC_A2

$9304.721 + 124.721589\ T - 24.348\ T \ln(T) - 2.53505E\text{-}3\ T^2 + 0.192818E\text{-}6\ T^3 + 32915\ T^{-1}$ *(298.15 < T < 1200)*

$1224.002 + 190.967426\ T - 33.586\ T \ln(T) + 2.24565E\text{-}3\ T^2 - 0.281835E\text{-}6\ T^3 + 1376270\ T^{-1}$ *(1200 < T < 2400)*

$-53882.739 + 458.410749\ T - 67.956\ T \ln(T) + 11.84945E\text{-}3\ T^2 - 0.788955E\text{-}6\ T^3 + 18075200\ T^{-1}$ *(2400 < T < 3458)*

$363325.888 - 1215.071859\ T + 140.8316548\ T \ln(T) - 33.764567E\text{-}3\ T^2 + 1.053726E\text{-}6\ T^3 - 134548866\ T^{-1}$ *(3458 < T < 5000)*

$-61564.296 + 343.297842\ T - 49.519\ T \ln(T)$ *(5000 < T < 6000)*

FCC_A1

$3304.721 + 126.921589\ T - 24.348\ T \ln(T) - 2.53505E\text{-}3\ T^2 + 0.192818E\text{-}6\ T^3 + 32915\ T^{-1}$ *(298.15 < T < 1200)*

$-4775.998 + 193.167426\ T - 33.586\ T \ln(T) + 2.24565E\text{-}3\ T^2 - 0.281835E\text{-}6\ T^3 + 1376270\ T^{-1}$ *(1200 < T < 2400)*

$-59882.739 + 460.610749\ T - 67.956\ T \ln(T) + 11.84945E\text{-}3\ T^2 - 0.788955E\text{-}6\ T^3 + 18075200\ T^{-1}$ *(2400 < T < 3458)*

$357325.888 - 1212.871859\ T + 140.8316548\ T \ln(T) - 33.764567E\text{-}3\ T^2 + 1.053726E\text{-}6\ T^3 - 134548866\ T^{-1}$ *(3458 < T < 5000)*

$-67564.296 + 345.497842\ T - 49.519\ T \ln(T)$ *(5000 < T < 6000)*

Data relative to HCP_A3

LIQUID

$23820.883 - 6.34538\ T$ *(298.15 < T < 2000)*

$584618.663 - 2722.505881\ T + 347.7648975\ T \ln(T) - 91.64382E\text{-}3\ T^2 + 4.210375E\text{-}6\ T^3 - 164477257\ T^{-1}$ *(2000 < T < 2400)*

$639725.404 - 2989.949204\ T + 382.1348975\ T \ln(T) - 101.24762E\text{-}3\ T^2 + 4.717495E\text{-}6\ T^3 - 181176187\ T^{-1}$ *(2400 < T < 3458)*

$-385370.776 + 1547.09555\ T - 190.3506548\ T \ln(T) + 33.764567E\text{-}3\ T^2 - 1.053726E\text{-}6\ T^3 + 134548866\ T^{-1}$ *(3458 < T < 5000)*

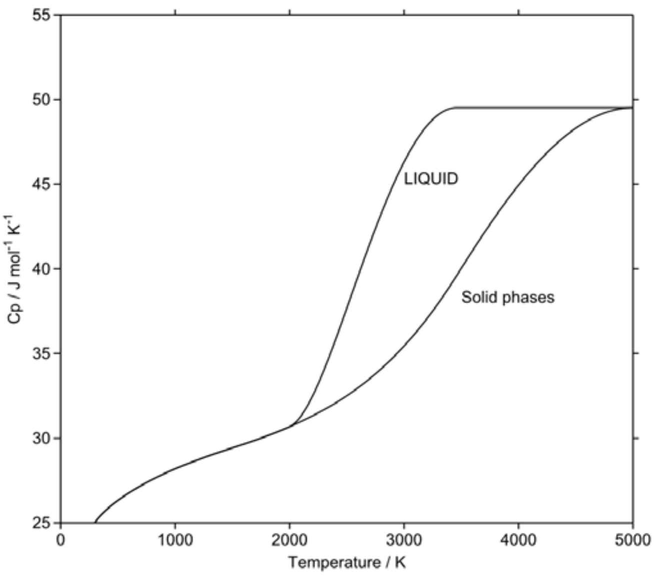
$39519.408 - 11.274151\ T$ *(5000 < T < 6000)*

BCC_A2

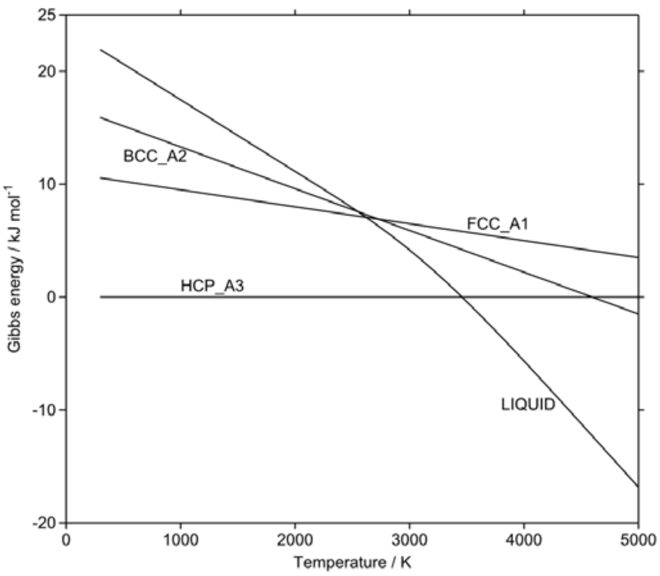
$17000 - 3.7\ T$ *(298.15 < T < 6000)*

FCC_A1

$11000 - 1.5\ T$ *(298.15 < T < 6000)*



Heat capacity of Re



Gibbs energy of phases of Re relative to HCP_A3

Rh

Source of data: *L.B. Pankratz, Bureau of Mines Bull. 672 [FCC_A1, LIQUID]*
Saunders et al. [HCP_A3, BCC_A2]

FCC_A1

$-7848.828 + 132.020923\ T - 24.0178336\ T \ln(T) - 3.424186E\text{-}3\ T^2 - 0.168032E\text{-}6\ T^3 + 55846\ T^{-1}$ *(298.15 < T < 1200)*

$-28367.852 + 305.771019\ T - 48.3766632\ T \ln(T) + 9.66345E\text{-}3\ T^2 - 1.512774E\text{-}6\ T^3 + 3348162\ T^{-1}$ *(1200 < T < 2237)*

$-6237470.481 + 30151.634226\ T - 3874.2105805\ T \ln(T) + 1049.213607E\text{-}3\ T^2 - 53.978814E\text{-}6\ T^3 + 1880362184\ T^{-1}$ *(2237 < T < 2450)*

$-44863.489 + 344.889895\ T - 50.58456\ T \ln(T)$ *(2450 < T < 2500)*

LIQUID

$11244.082 + 125.099593\ T - 24.0178336\ T \ln(T) - 3.424186E\text{-}3\ T^2 - 0.168032E\text{-}6\ T^3 + 55846\ T^{-1}$ *(298.15 < T < 700)*

$35898.508 - 147.926418\ T + 15.6492377\ T \ln(T) - 28.665357E\text{-}3\ T^2 + 2.100572E\text{-}6\ T^3 - 2638940\ T^{-1}$ *(700 < T < 2237)*

$-18208.54 + 332.974832\ T - 50.58456\ T \ln(T)$ *(2237 < T < 2500)*

BCC_A2

$11151.172 + 127.320923\ T - 24.0178336\ T \ln(T) - 3.424186E\text{-}3\ T^2 - 0.168032E\text{-}6\ T^3 + 55846\ T^{-1}$ *(298.15 < T < 1200)*

$-9367.852 + 301.071019\ T - 48.3766632\ T \ln(T) + 9.66345E\text{-}3\ T^2 - 1.512774E\text{-}6\ T^3 + 3348162\ T^{-1}$ *(1200 < T < 2237)*

$-6218470.481 + 30146.934226\ T - 3874.2105805\ T \ln(T) + 1049.213607E{-3}\ T^2 - 53.978814E{-6}\ T^3 + 1880362184\ T^{-1}$ *(2237 < T < 2450)*

$-25863.489 + 340.189895\ T - 50.58456\ T \ln(T)$ *(2450 < T < 2500)*

HCP_A3

$-4848.828 + 131.520923\ T - 24.0178336\ T \ln(T) - 3.424186E{-3}\ T^2 - 0.168032E{-6}\ T^3 + 55846\ T^{-1}$ *(298.15 < T < 1200)*

$-25367.852 + 305.271019\ T - 48.3766632\ T \ln(T) + 9.66345E{-3}\ T^2 - 1.512774E{-6}\ T^3 + 3348162\ T^{-1}$ *(1200 < T < 2237)*

$-6234470.481 + 30151.134226\ T - 3874.2105805\ T \ln(T) + 1049.213607E{-3}\ T^2 - 53.978814E{-6}\ T^3 + 1880362184\ T^{-1}$ *(2237 < T < 2450)*

$-41863.489 + 344.389895\ T - 50.58456\ T \ln(T)$ *(2450 < T < 2500)*

Data relative to FCC_A1

LIQUID

$19092.91 - 6.92133\ T$ *(298.15 < T < 700)*

$43747.336 - 279.947341\ T + 39.6670713\ T \ln(T) - 25.241171E{-3}\ T^2 + 2.268604E{-6}\ T^3 - 2694786\ T^{-1}$ *(700 < T < 1200)*

$64266.36 - 453.697437\ T + 64.0259009\ T \ln(T) - 38.328807E{-3}\ T^2 + 3.613346E{-6}\ T^3 - 5987102\ T^{-1}$ *(1200 < T < 2237)*

$6219261.941 - 29818.659394\ T + 3823.6260205\ T \ln(T) - 1049.213607E{-3}\ T^2 + 53.978814E{-6}\ T^3 - 1880362184\ T^{-1}$ *(2237 < T < 2450)*

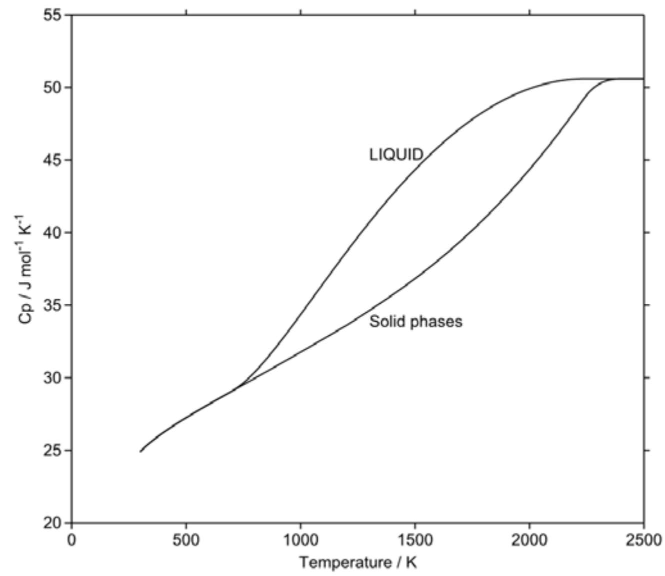
$26654.949 - 11.915063\ T$ *(2450 < T < 2500)*

BCC_A2

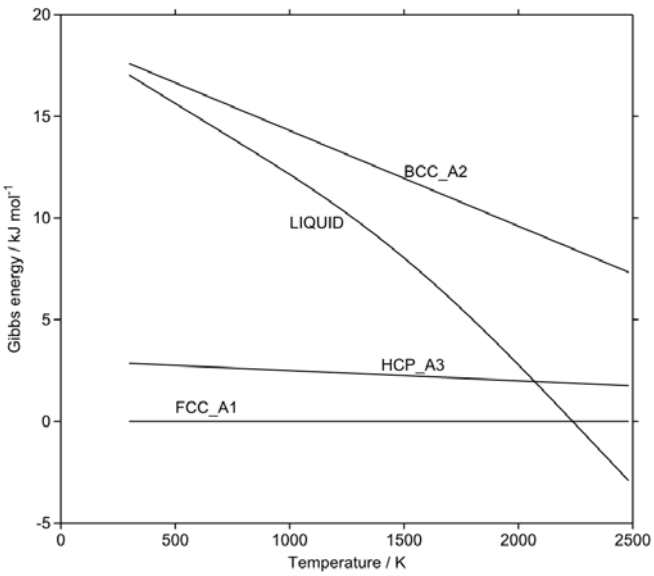
$19000 - 4.7\ T$ *(298.15 < T < 2500)*

HCP_A3

$3000 - 0.5\ T$ *(298.15 < T < 2500)*



Heat capacity of Rh



Gibbs energy of phases of Rh relative to FCC_A1

Ru

Source of data: *L B Pankratz, Bureau of Mines Bull. 672, revised by M H Rand [HCP_A3, LIQUID]*
Saunders et al. [FCC_A1]
A T Dinsdale (unpublished, 2000) [BCC_A2]

HCP_A3

$-7561.873 + 127.866233\ T - 22.9143287\ T\ln(T) - 4.062566\text{E-}3\ T^2 + 0.17641\text{E-}6\ T^3 + 56377\ T^{-1}$ *(298.15 < T < 1500)*

$-59448.103 + 489.516214\ T - 72.3241219\ T\ln(T) + 18.726245\text{E-}3\ T^2 - 1.952433\text{E-}6\ T^3 + 11063885\ T^{-1}$ *(1500 < T < 2607)*

$-38588773.031 + 168610.517401\ T - 21329.7050475\ T\ln(T) + 5221.638997\text{E-}3\ T^2 - 240.245985\text{E-}6\ T^3 + 13082992629\ T^{-1}$ *(2607 < T < 2740)*

$-55768.304 + 364.482314\ T - 51.8816\ T\ln(T)$ *(2740 < T < 4500)*

LIQUID

$19918.743 + 119.467485\ T - 22.9143287\ T\ln(T) - 4.062566\text{E-}3\ T^2 + 0.17641\text{E-}6\ T^3 + 56377\ T^{-1}$ *(298.15 < T < 800)*

$50827.232 - 179.818561\ T + 19.539341\ T\ln(T) - 26.524167\text{E-}3\ T^2 + 1.667839\text{E-}6\ T^3 - 3861125\ T^{-1}$ *(800 < T < 2607)*

$-17161.807 + 349.673561\ T - 51.8816\ T\ln(T)$ *(2607 < T < 4500)*

BCC_A2

$13938.127 + 122.816233\ T - 22.9143287\ T\ln(T) - 4.062566\text{E-}3\ T^2 + 0.17641\text{E-}6\ T^3 + 56377\ T^{-1}$ *(298.15 < T < 1500)*

$-37948.103 + 484.466214\ T - 72.3241219\ T\ln(T) + 18.726245E\text{-}3\ T^2 - 1.952433E\text{-}6\ T^3 + 11063885\ T^{-1}$ *(1500 < T < 2607)*

$-38567273.031 + 168605.467401\ T - 21329.7050475\ T\ln(T) + 5221.638997E\text{-}3\ T^2 - 240.245985E\text{-}6\ T^3 + 13082992629\ T^{-1}$ *(2607 < T < 2740)*

$-34268.304 + 359.432314\ T - 51.8816\ T\ln(T)$ *(2740 < T < 4500)*

FCC_A1

$4938.127 + 125.466233\ T - 22.9143287\ T\ln(T) - 4.062566E\text{-}3\ T^2 + 0.17641E\text{-}6\ T^3 + 56377\ T^{-1}$ *(298.15 < T < 1500)*

$-46948.103 + 487.116214\ T - 72.3241219\ T\ln(T) + 18.726245E\text{-}3\ T^2 - 1.952433E\text{-}6\ T^3 + 11063885\ T^{-1}$ *(1500 < T < 2607)*

$-38576273.031 + 168608.117401\ T - 21329.7050475\ T\ln(T) + 5221.638997E\text{-}3\ T^2 - 240.245985E\text{-}6\ T^3 + 13082992629\ T^{-1}$ *(2607 < T < 2740)*

$-43268.304 + 362.082314\ T - 51.8816\ T\ln(T)$ *(2740 < T < 4500)*

Data relative to HCP_A3

LIQUID

$27480.616 - 8.398748\ T$ *(298.15 < T < 800)*

$58389.105 - 307.684794\ T + 42.4536697\ T\ln(T) - 22.461601E\text{-}3\ T^2 + 1.491429E\text{-}6\ T^3 - 3917502\ T^{-1}$ *(800 < T < 1500)*

$110275.335 - 669.334775\ T + 91.8634629\ T\ln(T) - 45.250412E\text{-}3\ T^2 + 3.620272E\text{-}6\ T^3 - 14925010\ T^{-1}$ *(1500 < T < 2607)*

$38571611.224 - 168260.84384\ T + 21277.8234475\ T\ln(T) - 5221.638997E\text{-}3\ T^2 + 240.245985E\text{-}6\ T^3 - 13082992629\ T^{-1}$ *(2607 < T < 2740)*

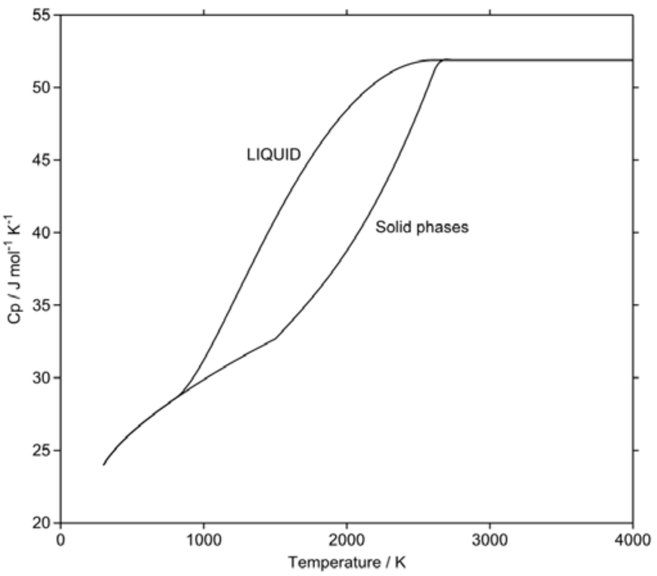
$38606.497 - 14.808753\ T$ *(2740 < T < 4500)*

BCC_A2

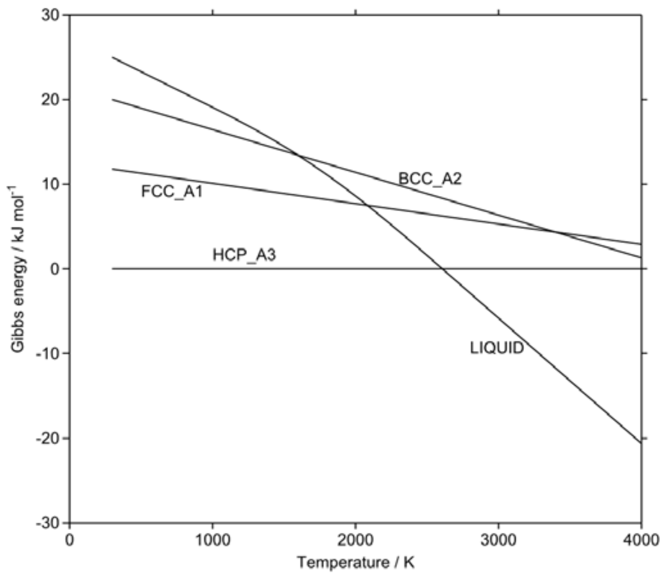
$21500 - 5.05\ T$ *(298.15 < T < 4500)*

FCC_A1

$12500 - 2.4\ T$ *(298.15 < T < 4500)*



Heat capacity of Ru



Gibbs energy of phases of Ru relative to HCP_A3

S

Source of data: *TPIS [ORTHORHOMBIC_S, MONOCLINIC, LIQUID]*
Sundman, (Unpublished work) [FCC_A1, BCC_A2]

ORTHORHOMBIC_S

$-5198.294 + 53.913855\ T - 10.726\ T\ \ln(T) - 27.3801E\text{-}3\ T^2 + 8.179537E\text{-}6\ T^3$ *(298.15 < T < 368.3)*
$-6475.706 + 94.182332\ T - 17.8693298\ T\ \ln(T) - 10.936877E\text{-}3\ T^2 + 1.406467E\text{-}6\ T^3 + 36871\ T^{-1}$ *(368.3 < T < 1300)*
$-12485.546 + 188.304687\ T - 32\ T\ \ln(T)$ *(1300 < T < 1301)*

MONOCLINIC

$-5725.422 + 89.544275\ T - 17.413\ T\ \ln(T) - 9.93935E\text{-}3\ T^2 - 0.070062E\text{-}6\ T^3 + 1250\ T^{-1}$ *(298.15 < T < 388.36)*
$-7455.008 + 114.782945\ T - 21.1531404\ T\ \ln(T) - 8.566163E\text{-}3\ T^2 + 1.112484E\text{-}6\ T^3 + 122167\ T^{-1}$ *(388.36 < T < 1300)*
$-11779.415 + 186.699065\ T - 32\ T\ \ln(T)$ *(1300 < T < 1301)*

LIQUID

$-4196.575 + 85.63027\ T - 17.413\ T\ \ln(T) - 9.93935E\text{-}3\ T^2 - 0.070062E\text{-}6\ T^3 + 1250\ T^{-1}$ *(298.15 < T < 335)*
$1790361.982 - 44195.451432\ T + 7511.6194258\ T\ \ln(T) - 13985.517511E\text{-}3\ T^2 + 4838.738601E\text{-}6\ T^3 - 79880891\ T^{-1}$ *(335 < T < 388.36)*
$-876313.954 + 23366.872986\ T - 4028.756\ T\ \ln(T) + 7954.595E\text{-}3\ T^2 - 2908.513333E\text{-}6\ T^3 + 33980035\ T^{-1}$ *(388.36 < T < 432.25)*

$454088.687 - 7814.670231\ T + 1237.001\ T \ln(T) - 1560.7295E\text{-}3\ T^2 + 359.883667E\text{-}6\ T^3$
$- 31765395\ T^{-1}$ *(432.25 < T < 500)*

$18554.561 - 144.895285\ T + 16.535\ T \ln(T) - 45.4119E\text{-}3\ T^2 + 8.327402E\text{-}6\ T^3 - 2705030\ T^{-1}$
(500 < T < 700)

$21243.126 - 113.298877\ T + 9.944\ T \ln(T) - 28.8384E\text{-}3\ T^2 + 3.791365E\text{-}6\ T^3 - 3507570\ T^{-1}$
(700 < T < 900)

$16117.849 - 32.79523\ T - 2.425\ T \ln(T) - 17.12545E\text{-}3\ T^2 + 1.84974E\text{-}6\ T^3 - 3215170\ T^{-1}$
(900 < T < 1300)

$-6461.814 + 175.590536\ T - 32\ T \ln(T)$ *(1300 < T < 1301)*

BCC_A2

$99801.706 + 53.913855\ T - 10.726\ T \ln(T) - 27.3801E\text{-}3\ T^2 + 8.179537E\text{-}6\ T^3$ *(298.15 < T < 368.3)*

$98524.294 + 94.182332\ T - 17.8693298\ T \ln(T) - 10.936877E\text{-}3\ T^2 + 1.406467E\text{-}6\ T^3 + 36871\ T^{-1}$
(368.3 < T < 1300)

$92514.454 + 188.304687\ T - 32\ T \ln(T)$ *(1300 < T < 1301)*

FCC_A1

$99801.706 + 53.913855\ T - 10.726\ T \ln(T) - 27.3801E\text{-}3\ T^2 + 8.179537E\text{-}6\ T^3$ *(298.15 < T < 368.3)*

$98524.294 + 94.182332\ T - 17.8693298\ T \ln(T) - 10.936877E\text{-}3\ T^2 + 1.406467E\text{-}6\ T^3 + 36871\ T^{-1}$
(368.3 < T < 1300)

$92514.454 + 188.304687\ T - 32\ T \ln(T)$ *(1300 < T < 1301)*

Data relative to ORTHORHOMBIC_S

MONOCLINIC

$-527.128 + 35.63042\ T - 6.687\ T \ln(T) + 17.44075E\text{-}3\ T^2 - 8.249599E\text{-}6\ T^3 + 1250\ T^{-1}$
(298.15 < T < 368.3)

$750.284 - 4.638057\ T + 0.4563298\ T \ln(T) + 0.997527E\text{-}3\ T^2 - 1.476529E\text{-}6\ T^3 - 35621\ T^{-1}$
(368.3 < T < 388.36)

$-979.302 + 20.600613\ T - 3.2838106\ T \ln(T) + 2.370714E\text{-}3\ T^2 - 0.293983E\text{-}6\ T^3 + 85296\ T^{-1}$
(388.36 < T < 1300)

$706.131 - 1.605622\ T$ *(1300 < T < 1301)*

LIQUID

$1001.719 + 31.716415\ T - 6.687\ T \ln(T) + 17.44075E\text{-}3\ T^2 - 8.249599E\text{-}6\ T^3 + 1250\ T^{-1}$
(298.15 < T < 335)

$1795560.276 - 44249.365287\ T + 7522.3454258\ T \ln(T) - 13958.137411E\text{-}3\ T^2 + 4830.559064E\text{-}6\ T^3$
$- 79880891\ T^{-1}$ *(335 < T < 368.3)*

$1796837.688 - 44289.633764\ T + 7529.4887556\ T \ln(T) - 13974.580634E\text{-}3\ T^2 + 4837.332134E\text{-}6\ T^3$
$- 79917762\ T^{-1}$ *(368.3 < T < 388.36)*

$-869838.248 + 23272.690654\ T - 4010.8866702\ T \ln(T) + 7965.531877E\text{-}3\ T^2 - 2909.9198E\text{-}6\ T^3$
$+ 33943164\ T^{-1}$ *(388.36 < T < 432.25)*

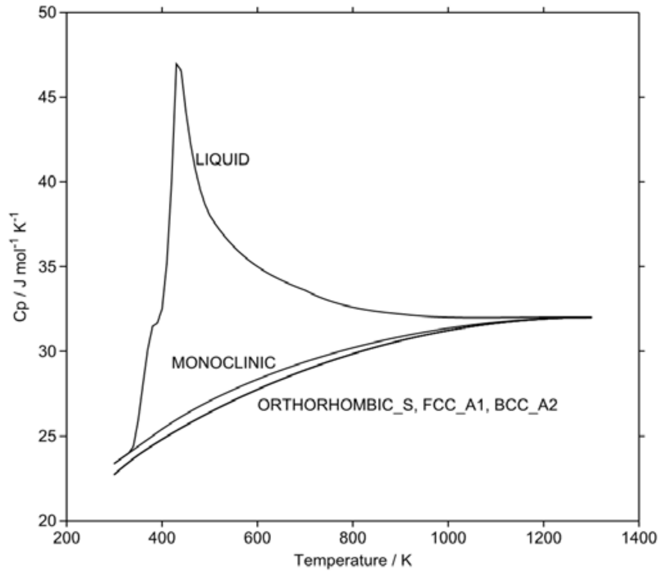
$460564.393 - 7908.852563\ T + 1254.8703298\ T\ \ln(T) - 1549.792623E\text{-}3\ T^{2} + 358.4772E\text{-}6\ T^{3}$
$- 31802266\ T^{-1}$ *(432.25 < T < 500)*
$25030.267 - 239.077617\ T + 34.4043298\ T\ \ln(T) - 34.475023E\text{-}3\ T^{2} + 6.920935E\text{-}6\ T^{3} - 2741901\ T^{-1}$
(500 < T < 700)
$27718.832 - 207.481209\ T + 27.8133298\ T\ \ln(T) - 17.901523E\text{-}3\ T^{2} + 2.384898E\text{-}6\ T^{3} - 3544441\ T^{-1}$
(700 < T < 900)
$22593.555 - 126.977562\ T + 15.4443298\ T\ \ln(T) - 6.188573E\text{-}3\ T^{2} + 0.443273E\text{-}6\ T^{3} - 3252041\ T^{-1}$
(900 < T < 1300)
$6023.732 - 12.714151\ T$ *(1300 < T < 1301)*

BCC_A2

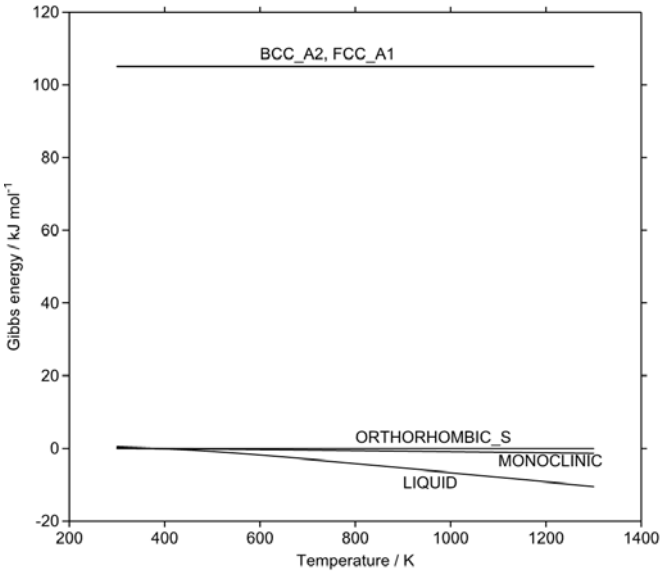
105000 *(298.15 < T < 1301)*

FCC_A1

105000 *(298.15 < T < 1301)*



Heat capacity of S



Gibbs energy of phases of S relative to ORTHORHOMBIC_S

Sb

Source of data: *Hultgren [RHOMBO_A7, LIQUID]*
Saunders et al. [FCC_A1, BCC_A2, HCP_A3]
A T Dinsdale (unpublished) [BCT_A5]

RHOMBOHEDRAL_A7

$-9242.858 + 156.154689\ T - 30.5130752\ T\ \ln(T) + 7.748768E\text{-}3\ T^{2} - 3.003415E\text{-}6\ T^{3} + 100625\ T^{-1}$
(298.15 < T < 903.78)

$-11738.83 + 169.485872\,T - 31.38\,T\ln(T) + 1616.849E24\,T^{-9}$ *(903.78 < T < 2000)*

LIQUID

$10579.47 + 134.231525\,T - 30.5130752\,T\ln(T) + 7.748768E{-3}\,T^{2} - 3.003415E{-6}\,T^{3} + 100625\,T^{-1}$
$- 174.847E{-22}\,T^{7}$ *(298.15 < T < 903.78)*
$8175.359 + 147.455986\,T - 31.38\,T\ln(T)$ *(903.78 < T < 2000)*

BCT_A5

$3757.142 + 148.154689\,T - 30.5130752\,T\ln(T) + 7.748768E{-3}\,T^{2} - 3.003415E{-6}\,T^{3} + 100625\,T^{-1}$
(298.15 < T < 903.78)
$1261.17 + 161.485872\,T - 31.38\,T\ln(T) + 1616.849E24\,T^{-9}$ *(903.78 < T < 2000)*

BCC_A2

$10631.142 + 141.054689\,T - 30.5130752\,T\ln(T) + 7.748768E{-3}\,T^{2} - 3.003415E{-6}\,T^{3} + 100625\,T^{-1}$
(298.15 < T < 903.78)
$8135.17 + 154.385872\,T - 31.38\,T\ln(T) + 1616.849E24\,T^{-9}$ *(903.78 < T < 2000)*

FCC_A1

$10631.142 + 142.454689\,T - 30.5130752\,T\ln(T) + 7.748768E{-3}\,T^{2} - 3.003415E{-6}\,T^{3} + 100625\,T^{-1}$
(298.15 < T < 903.78)
$8135.17 + 155.785872\,T - 31.38\,T\ln(T) + 1616.849E24\,T^{-9}$ *(903.78 < T < 2000)*

HCP_A3

$10631.142 + 143.154689\,T - 30.5130752\,T\ln(T) + 7.748768E{-3}\,T^{2} - 3.003415E{-6}\,T^{3} + 100625\,T^{-1}$
(298.15 < T < 903.78)
$8135.17 + 156.485872\,T - 31.38\,T\ln(T) + 1616.849E24\,T^{-9}$ *(903.78 < T < 2000)*

Data relative to RHOMBOHEDRAL_A7

LIQUID

$19822.328 - 21.923164\,T - 174.847E{-22}\,T^{7}$ *(298.15 < T < 903.78)*
$19914.189 - 22.029886\,T - 1616.849E24\,T^{-9}$ *(903.78 < T < 2000)*

BCT_A5

$13000 - 8\,T$ *(298.15 < T < 2000)*

BCC_A2

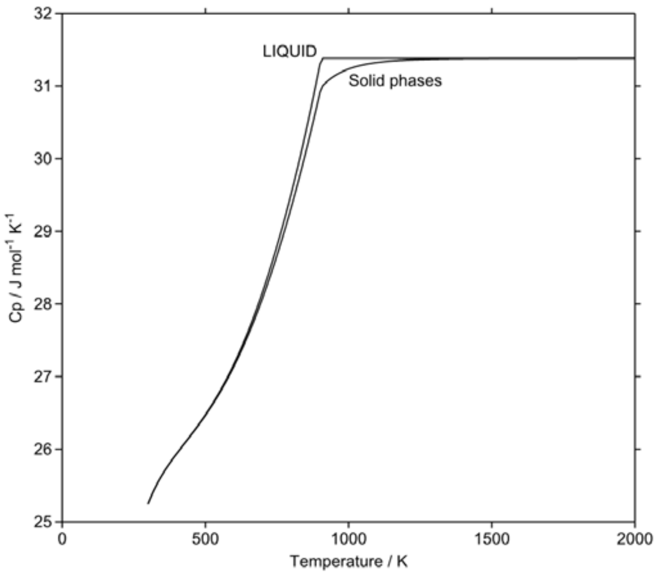
$19874 - 15.1\,T$ *(298.15 < T < 2000)*

FCC_A1

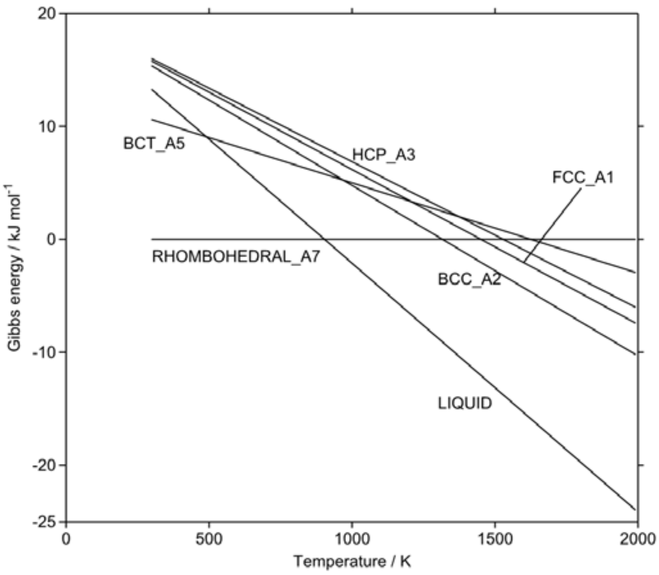
$19874 - 13.7\ T$ *(298.15 < T < 2000)*

HCP_A3

$19874 - 13\ T$ *(298.15 < T < 2000)*



Heat capacity of Sb



Gibbs energy of phases of Sb relative to RHOMBOHEDRAL_A7

Sc

Source of data: *Hultgren [HCP_A3, BCC_A2, LIQUID]*
G Cacciamani;P Riani; G Borzone; N Parodi; A Saccone; R Ferro; A Pisch; R Schmid-Fetzer; Intermetallics, 7 (1), 101-108 (1999) [FCC_A1]
S Norgren, Thesis, Royal Institute of Technology Stockholm, 2000 [DHCP]

HCP_A3

$-8689.547 + 153.48097\ T - 28.1882\ T\ln(T) + 3.21892E\text{-}3\ T^2 - 1.64531E\text{-}6\ T^3 + 72177\ T^{-1}$ *(298.15 < T < 800)*

$-7511.295 + 132.759582\ T - 24.9132\ T\ln(T) - 0.573295E\text{-}3\ T^2 - 0.859345E\text{-}6\ T^3$ *(800 < T < 1608)*

$261143.04 - 1817.922454\ T + 241.4410508\ T\ln(T) - 117.529396E\text{-}3\ T^2 + 8.7398E\text{-}6\ T^3 - 50607159\ T^{-1}$ *(1608 < T < 2000)*

$-30515.246 + 286.474338\ T - 44.2249\ T\ln(T)$ *(2000 < T < 3200)*

BCC_A2

$-6709.819 + 152.456835\ T - 28.1882\ T\ln(T) + 3.21892E\text{-}3\ T^2 - 1.64531E\text{-}6\ T^3 + 72177\ T^{-1}$ *(298.15 < T < 800)*

$-5531.567 + 131.735447\ T - 24.9132\ T\ln(T) - 0.573295E\text{-}3\ T^2 - 0.859345E\text{-}6\ T^3$ *(800 < T < 1000)*
$230161.408 - 2004.054685\ T + 276.7666402\ T\ln(T) - 167.120107E\text{-}3\ T^2 + 15.637371E\text{-}6\ T^3$
$- 33783257\ T^{-1}$ *(1000 < T < 1608)*
$-25928.011 + 283.642312\ T - 44.2249\ T\ln(T)$ *(1608 < T < 3200)*

LIQUID

$6478.66 + 45.427539\ T - 10.7967803\ T\ln(T) - 20.636524E\text{-}3\ T^2 + 2.13106E\text{-}6\ T^3 - 158106\ T^{-1}$
(298.15 < T < 1608)
$-11832.111 + 275.871695\ T - 44.2249\ T\ln(T)$ *(1608 < T < 3200)*

DHCP

$-7489.547 + 153.896695\ T - 28.1882\ T\ln(T) + 3.21892E\text{-}3\ T^2 - 1.64531E\text{-}6\ T^3 + 72177\ T^{-1}$
(298.15 < T < 800)
$-6311.295 + 133.175308\ T - 24.9132\ T\ln(T) - 0.573295E\text{-}3\ T^2 - 0.859345E\text{-}6\ T^3$ *(800 < T < 1608)*
$262343.04 - 1817.506729\ T + 241.4410508\ T\ln(T) - 117.529396E\text{-}3\ T^2 + 8.7398E\text{-}6\ T^3 - 50607159\ T^{-1}$
(1608 < T < 2000)
$-29315.246 + 286.890063\ T - 44.2249\ T\ln(T)$ *(2000 < T < 3200)*

FCC_A1

$-3689.547 + 153.48097\ T - 28.1882\ T\ln(T) + 3.21892E\text{-}3\ T^2 - 1.64531E\text{-}6\ T^3 + 72177\ T^{-1}$
(298.15 < T < 800)
$-2511.295 + 132.759582\ T - 24.9132\ T\ln(T) - 0.573295E\text{-}3\ T^2 - 0.859345E\text{-}6\ T^3$ *(800 < T < 1608)*
$266143.04 - 1817.922454\ T + 241.4410508\ T\ln(T) - 117.529396E\text{-}3\ T^2 + 8.7398E\text{-}6\ T^3 - 50607159\ T^{-1}$
(1608 < T < 2000)
$-25515.246 + 286.474338\ T - 44.2249\ T\ln(T)$ *(2000 < T < 3200)*

Data relative to HCP_A3

BCC_A2

$1979.728 - 1.024135\ T$ *(298.15 < T < 1000)*
$237672.703 - 2136.814267\ T + 301.6798402\ T\ln(T) - 166.546812E\text{-}3\ T^2 + 16.496716E\text{-}6\ T^3$
$- 33783257\ T^{-1}$ *(1000 < T < 1608)*
$-287071.051 + 2101.564766\ T - 285.6659508\ T\ln(T) + 117.529396E\text{-}3\ T^2 - 8.7398E\text{-}6\ T^3$
$+ 50607159\ T^{-1}$ *(1608 < T < 2000)*
$4587.235 - 2.832026\ T$ *(2000 < T < 3200)*

LIQUID

$15168.207 - 108.053431\ T + 17.3914197\ T\ln(T) - 23.855444E\text{-}3\ T^2 + 3.77637E\text{-}6\ T^3 - 230283\ T^{-1}$
(298.15 < T < 800)
$13989.955 - 87.332043\ T + 14.1164197\ T\ln(T) - 20.063229E\text{-}3\ T^2 + 2.990405E\text{-}6\ T^3 - 158106\ T^{-1}$
(800 < T < 1608)

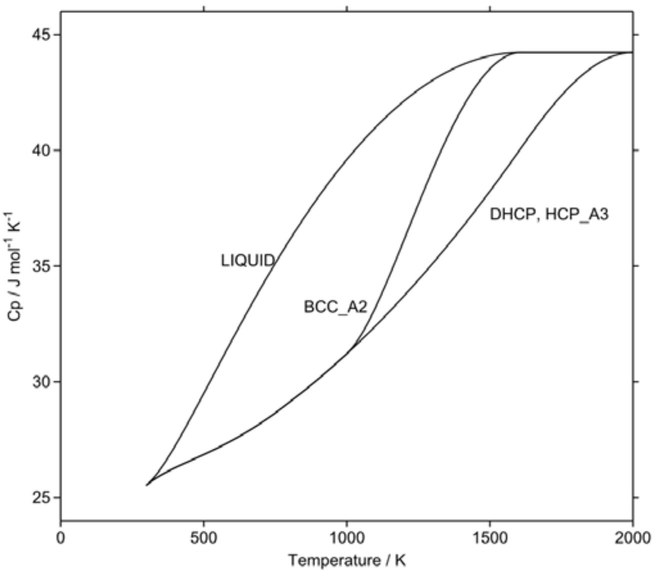
$-272975.151 + 2093.794149\ T - 285.6659508\ T\ \ln(T) + 117.529396E\text{-}3\ T^2 - 8.7398E\text{-}6\ T^3$
$+ 50607159\ T^{-1}$ *(1608 < T < 2000)*
$18683.135 - 10.602643\ T$ *(2000 < T < 3200)*

DHCP

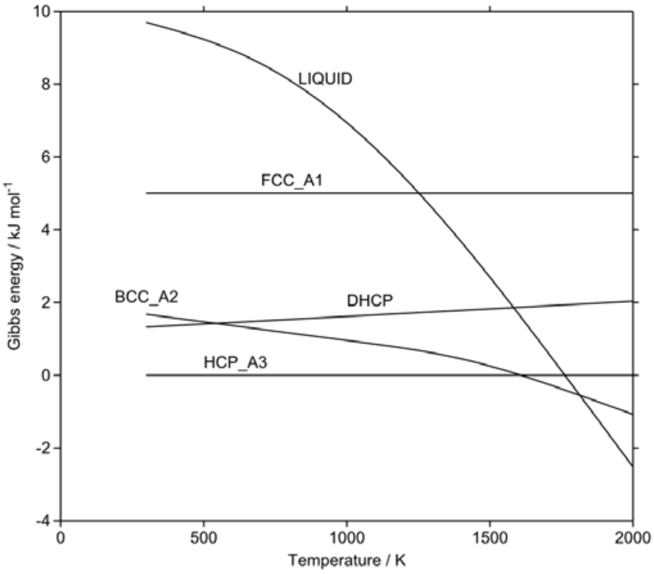
$1200 + 0.415725\ T$ *(298.15 < T < 3200)*

FCC_A1

5000 *(298.15 < T < 3200)*



Heat capacity of Sc



Gibbs energy of phases of Sc relative to HCP_A3

Se

Source of data: *Hultgren*

HEXAGONAL_A8

$-9376.371 + 174.205877\ T - 33.6527\ T\ \ln(T) + 24.24314E\text{-}3\ T^2 - 15.318461E\text{-}6\ T^3 + 102249\ T^{-1}$
(298.15 < T < 494)
$-37546.134 + 507.111538\ T - 81.2006585\ T\ \ln(T) + 37.144892E\text{-}3\ T^2 - 5.611026E\text{-}6\ T^3 + 2614263\ T^{-1}$
(494 < T < 800)
$-12193.47 + 197.770166\ T - 35.1456\ T\ \ln(T)$ *(800 < T < 1000)*

LIQUID

$50533.347 - 1178.288242\ T + 194.1074389\ T\ \ln(T) - 390.268991E\text{-}3\ T^2 + 119.219297E\text{-}6\ T^3$
$- 2224398\ T^{-1}$ *(298.15 < T < 494)*
$-5228.304 + 183.72559\ T - 35.1456\ T\ \ln(T)$ *(494 < T < 1000)*

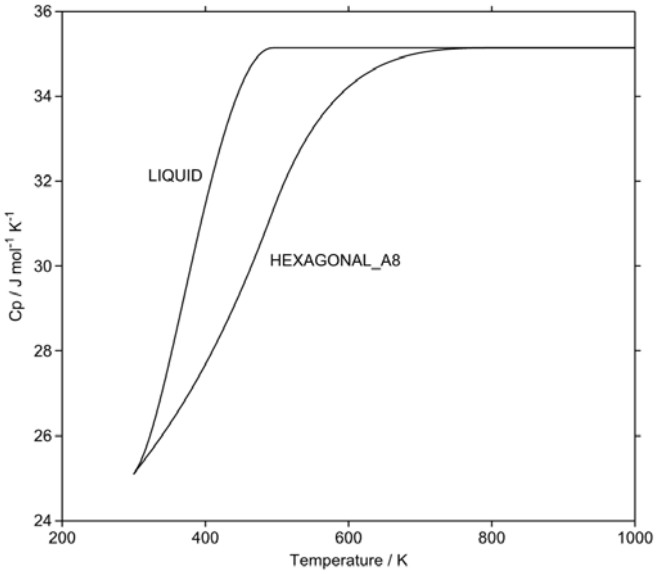
Data relative to HEXAGONAL_A8

LIQUID

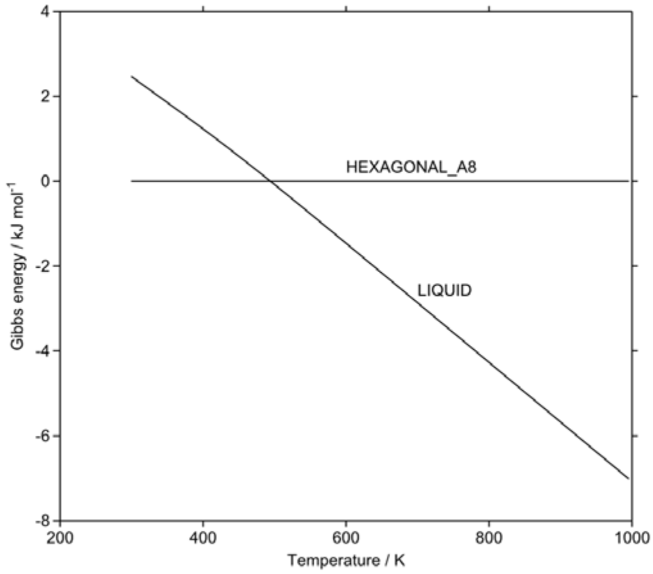
$59909.718 - 1352.494119\ T + 227.7601389\ T\ln(T) - 414.512131E\text{-}3\ T^2 + 134.537758E\text{-}6\ T^3 - 2326647\ T^{-1}$ *(298.15 < T < 494)*

$32317.83 - 323.385948\ T + 46.0550585\ T\ln(T) - 37.144892E\text{-}3\ T^2 + 5.611026E\text{-}6\ T^3 - 2614263\ T^{-1}$ *(494 < T < 800)*

$6965.166 - 14.044576\ T$ *(800 < T < 1000)*



Heat capacity of Se



Gibbs energy of phases of Se relative to HEXAGONAL_A8

Si

Source of data: *JANAF [DIAMOND_A4, LIQUID]*
Saunders et al. [BCC_A2, FCC_A1, HCP_A3]
Kaufman [BCC_A12, CUB_A13]

DIAMOND_A4

$-8162.609 + 137.236859\ T - 22.8317533\ T\ln(T) - 1.912904E\text{-}3\ T^2 - 0.003552E\text{-}6\ T^3 + 176667\ T^{-1}$ *(298.15 < T < 1687)*

$-9457.642 + 167.281367\ T - 27.196\ T\ln(T) - 420.369E28\ T^{-9}$ *(1687 < T < 3600)*

LIQUID

$42533.751 + 107.13742\ T - 22.8317533\ T\ln(T) - 1.912904E\text{-}3\ T^2 - 0.003552E\text{-}6\ T^3 + 176667\ T^{-1} + 209.307E\text{-}23\ T^7$ *(298.15 < T < 1687)*

$40370.523 + 137.722298\ T - 27.196\ T\ln(T)$ *(1687 < T < 3600)*

BCC_A2

$38837.391 + 114.736859\ T - 22.8317533\ T\ \ln(T) - 1.912904E{-3}\ T^2 - 0.003552E{-6}\ T^3 + 176667\ T^{-1}$ *(298.15 < T < 1687)*

$37542.358 + 144.781367\ T - 27.196\ T\ \ln(T) - 420.369E28\ T^{-9}$ *(1687 < T < 3600)*

CBCC_A12

$42045.391 + 116.859859\ T - 22.8317533\ T\ \ln(T) - 1.912904E{-3}\ T^2 - 0.003552E{-6}\ T^3 + 176667\ T^{-1}$ *(298.15 < T < 1687)*

$40750.358 + 146.904367\ T - 27.196\ T\ \ln(T) - 420.369E28\ T^{-9}$ *(1687 < T < 3600)*

CUB_A13

$39116.391 + 116.859859\ T - 22.8317533\ T\ \ln(T) - 1.912904E{-3}\ T^2 - 0.003552E{-6}\ T^3 + 176667\ T^{-1}$ *(298.15 < T < 1687)*

$37821.358 + 146.904367\ T - 27.196\ T\ \ln(T) - 420.369E28\ T^{-9}$ *(1687 < T < 3600)*

FCC_A1

$42837.391 + 115.436859\ T - 22.8317533\ T\ \ln(T) - 1.912904E{-3}\ T^2 - 0.003552E{-6}\ T^3 + 176667\ T^{-1}$ *(298.15 < T < 1687)*

$41542.358 + 145.481367\ T - 27.196\ T\ \ln(T) - 420.369E28\ T^{-9}$ *(1687 < T < 3600)*

HCP_A3

$41037.391 + 116.436859\ T - 22.8317533\ T\ \ln(T) - 1.912904E{-3}\ T^2 - 0.003552E{-6}\ T^3 + 176667\ T^{-1}$ *(298.15 < T < 1687)*

$39742.358 + 146.481367\ T - 27.196\ T\ \ln(T) - 420.369E28\ T^{-9}$ *(1687 < T < 3600)*

HCP_ZN

$41038.391 + 116.436859\ T - 22.8317533\ T\ \ln(T) - 1.912904E{-3}\ T^2 - 0.003552E{-6}\ T^3 + 176667\ T^{-1}$ *(298.15 < T < 1687)*

$39743.358 + 146.481367\ T - 27.196\ T\ \ln(T) - 420.369E28\ T^{-9}$ *(1687 < T < 3600)*

Data relative to DIAMOND_A4

LIQUID

$50696.36 - 30.099439\ T + 209.307E{-23}\ T^7$ *(298.15 < T < 1687)*

$49828.165 - 29.559069\ T + 420.369E28\ T^{-9}$ *(1687 < T < 3600)*

BCC_A2

$47000 - 22.5\ T$ *(298.15 < T < 3600)*

CBCC_A12

50208 - 20.377 T *(298.15 < T < 3600)*

CUB_A13

47279 - 20.377 T *(298.15 < T < 3600)*

FCC_A1

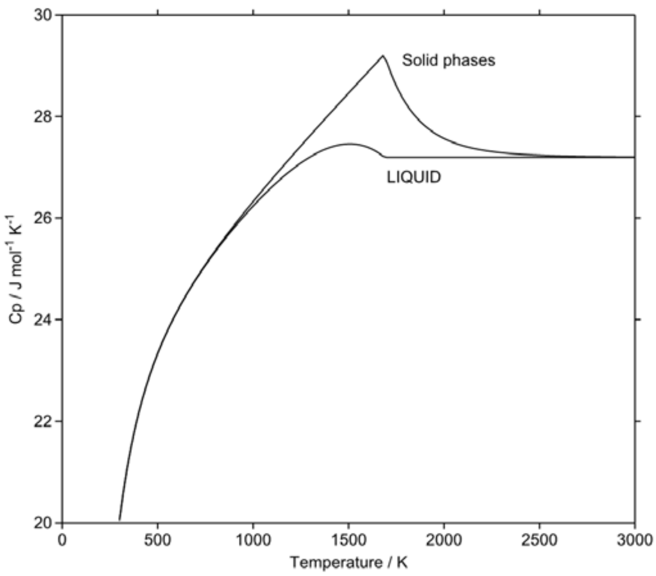
51000 - 21.8 T *(298.15 < T < 3600)*

HCP_A3

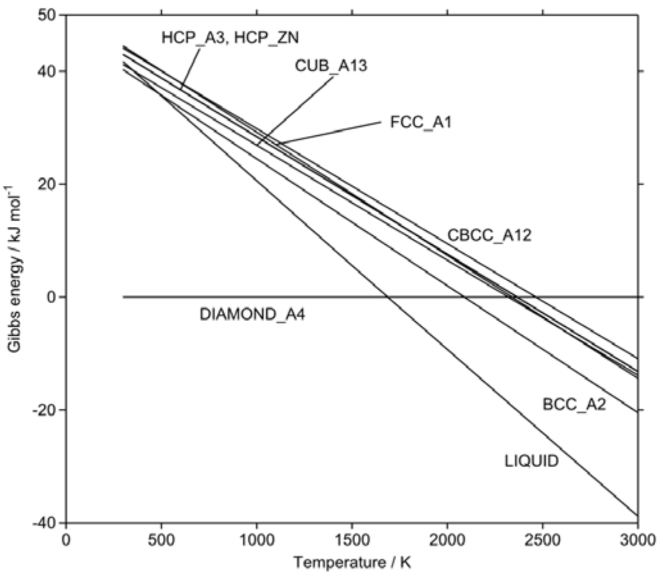
49200 - 20.8 T *(298.15 < T < 3600)*

HCP_ZN

49201 - 20.8 T *(298.15 < T < 3600)*



Heat capacity of Si



Gibbs energy of phases of Si relative to DIAMOND_A4

Sm

Source of data: *Hultgren [RHOMBO_C19, BCC_A2, LIQUID]*
Xuping Su, Weijing Zhang and Zhenmin Du; J. Alloys and Compounds 1998, 278, 182-4 [HCP_A3]

RHOMB_C19

$-3872.013 - 32.10748\ T - 1.6485\ T\ln(T) - 50.254E\text{-}3\ T^2 + 10.10345E\text{-}6\ T^3 - 82168\ T^{-1}$ *(298.15 < T < 700)*

$-50078.215 + 627.869894\ T - 102.665\ T\ln(T) + 47.4522E\text{-}3\ T^2 - 7.538383E\text{-}6\ T^3 + 3861770\ T^{-1}$ *(700 < T < 1190)*

$289719.819 - 2744.509764\ T + 381.4198202\ T\ln(T) - 254.986338E\text{-}3\ T^2 + 27.512152E\text{-}6\ T^3 - 40102102\ T^{-1}$ *(1190 < T < 1345)*

$-23056.079 + 282.194375\ T - 50.208\ T\ln(T)$ *(1345 < T < 2100)*

BCC_A2

$-4368.72 + 55.972523\ T - 16.9298494\ T\ln(T) - 25.446016E\text{-}3\ T^2 + 3.579527E\text{-}6\ T^3 + 94209\ T^{-1}$ *(298.15 < T < 1190)*

$-15957.862 + 253.121044\ T - 46.9445\ T\ln(T)$ *(1190 < T < 1345)*

$111191.653 - 624.680805\ T + 71.6856914\ T\ln(T) - 47.314968E\text{-}3\ T^2 + 3.329865E\text{-}6\ T^3 - 24870276\ T^{-1}$ *(1345 < T < 2100)*

HCP_A3

$-3802.036 - 32.176971\ T - 1.6485\ T\ln(T) - 50.254E\text{-}3\ T^2 + 10.10345E\text{-}6\ T^3 - 82168\ T^{-1}$ *(298.15 < T < 700)*

$-50008.238 + 627.800403\ T - 102.665\ T\ln(T) + 47.4522E\text{-}3\ T^2 - 7.538383E\text{-}6\ T^3 + 3861770\ T^{-1}$ *(700 < T < 1190)*

$289789.796 - 2744.579255\ T + 381.4198202\ T\ln(T) - 254.986338E\text{-}3\ T^2 + 27.512152E\text{-}6\ T^3 - 40102102\ T^{-1}$ *(1190 < T < 1345)*

$-22986.102 + 282.124884\ T - 50.208\ T\ln(T)$ *(1345 < T < 2100)*

LIQUID

$3468.783 + 20.117456\ T - 11.6968284\ T\ln(T) - 32.418177E\text{-}3\ T^2 + 4.544272E\text{-}6\ T^3 + 23528\ T^{-1}$ *(298.15 < T < 1190)*

$-11728.229 + 273.487076\ T - 50.208\ T\ln(T)$ *(1190 < T < 2100)*

Data relative to RHOMB_C19

BCC_A2

$-496.707 + 88.080003\ T - 15.2813494\ T\ln(T) + 24.807984E\text{-}3\ T^2 - 6.523923E\text{-}6\ T^3 + 176377\ T^{-1}$ *(298.15 < T < 700)*

$45709.495 - 571.897371\ T + 85.7351506\ T\ln(T) - 72.898216E\text{-}3\ T^2 + 11.11791E\text{-}6\ T^3 - 3767561\ T^{-1}$ *(700 < T < 1190)*

$-305677.681 + 2997.630808\ T - 428.3643202\ T\ln(T) + 254.986338E\text{-}3\ T^2 - 27.512152E\text{-}6\ T^3 + 40102102\ T^{-1}$ *(1190 < T < 1345)*

$134247.732 - 906.87518\ T + 121.8936914\ T\ln(T) - 47.314968E\text{-}3\ T^2 + 3.329865E\text{-}6\ T^3 - 24870276\ T^{-1}$ *(1345 < T < 2100)*

HCP_A3

$69.977 - 0.069491\ T$ *(298.15 < T < 2100)*

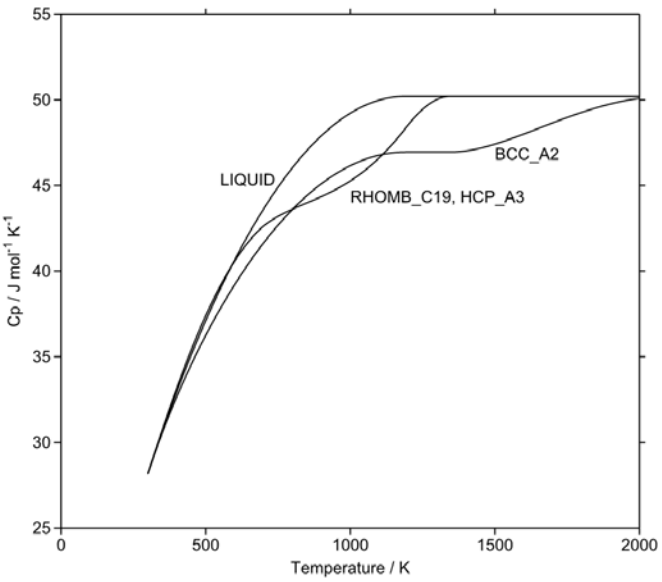
LIQUID

$7340.796 + 52.224936\ T - 10.0483284\ T\ln(T) + 17.835823E\text{-}3\ T^2 - 5.559178E\text{-}6\ T^3 + 105696\ T^{-1}$ *(298.15 < T < 700)*

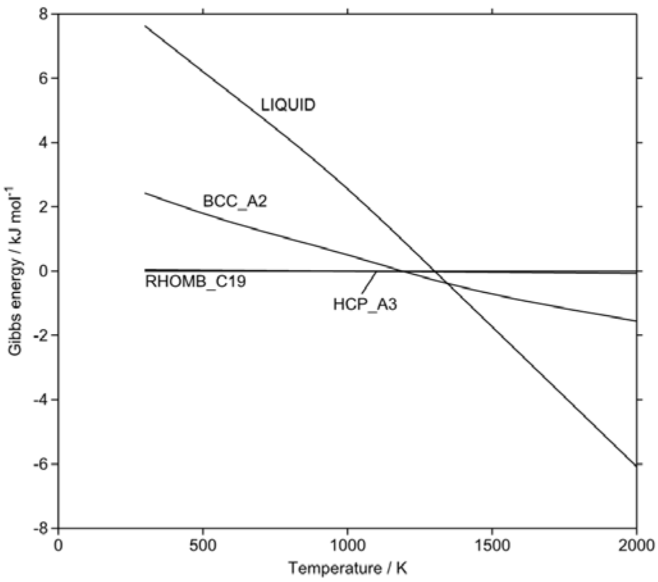
$53546.998 - 607.752438\ T + 90.9681716\ T\ln(T) - 79.870377E\text{-}3\ T^2 + 12.082655E\text{-}6\ T^3 - 3838242\ T^{-1}$ *(700 < T < 1190)*

$-301448.048 + 3017.99684\ T - 431.6278202\ T\ln(T) + 254.986338E\text{-}3\ T^2 - 27.512152E\text{-}6\ T^3 + 40102102\ T^{-1}$ *(1190 < T < 1345)*

$11327.85 - 8.707299\ T$ *(1345 < T < 2100)*



Heat capacity of Sm



Gibbs energy of phases of Sm relative to RHOMB_C19

Sn

Source of data: *Hultgren [BCT_A5, DIAMOND_A4, LIQUID]*
N Saunders et al. [BCC_A2]
I Ansara, unpublished work [HCP_A3, TETRAGONAL_A6, TET_ALPHA1]
H J Fecht, M X Zhang, Y A Chang, J H Perepezko;. Metall. Trans. A, 1989, 20A, 795-803 [FCC_A1]
J Miettinen, CALPHAD, 2004, 28(1), 71-77 [CBCC_A12, CUB_A13]
H S Liu; C L Liu; K Ishida; Z P Jin; J. Electron. Mater. 2033, 32, 1290 [DHCP]

BCT_A5

$-7958.517 + 122.765451\ T - 25.858\ T \ln(T) + 0.51185E\text{-}3\ T^2 - 3.192767E\text{-}6\ T^3 + 18440\ T^{-1}$ *(100 < T < 250)*

$-5855.135 + 65.443315\ T - 15.961\ T \ln(T) - 18.8702E\text{-}3\ T^2 + 3.121167E\text{-}6\ T^3 - 61960\ T^{-1}$ *(250 < T < 505.078)*

$2524.724 + 4.005269\ T - 8.2590486\ T \ln(T) - 16.814429E\text{-}3\ T^2 + 2.623131E\text{-}6\ T^3 - 1081244\ T^{-1} - 123.07E23\ T^{-9}$ *(505.078 < T < 800)*

$-8256.959 + 138.99688\ T - 28.4512\ T \ln(T) - 123.07E23\ T^{-9}$ *(800 < T < 3000)*

DIAMOND_A4

$-9579.608 + 114.007785\ T - 22.972\ T \ln(T) - 8.13975E\text{-}3\ T^2 + 2.7288E\text{-}6\ T^3 + 25615\ T^{-1}$ *(100 < T < 298.15)*

$-9063.001 + 104.84654\ T - 21.5750771\ T \ln(T) - 8.575282E\text{-}3\ T^2 + 1.784447E\text{-}6\ T^3 - 2544\ T^{-1}$ *(298.15 < T < 800)*

$-10909.351 + 147.396535\ T - 28.4512\ T \ln(T)$ *(800 < T < 3000)*

LIQUID

$-855.425 + 108.677684\ T - 25.858\ T \ln(T) + 0.51185E\text{-}3\ T^2 - 3.192767E\text{-}6\ T^3 + 18440\ T^{-1} + 147.031E\text{-}20\ T^7$ *(100 < T < 250)*

$1247.957 + 51.355548\ T - 15.961\ T \ln(T) - 18.8702E\text{-}3\ T^2 + 3.121167E\text{-}6\ T^3 - 61960\ T^{-1} + 147.031E\text{-}20\ T^7$ *(250 < T < 505.078)*

$9496.31 - 9.809114\ T - 8.2590486\ T \ln(T) - 16.814429E\text{-}3\ T^2 + 2.623131E\text{-}6\ T^3 - 1081244\ T^{-1}$ *(505.078 < T < 800)*

$-1285.372 + 125.182498\ T - 28.4512\ T \ln(T)$ *(800 < T < 3000)*

RHOMBOHEDRAL_A7

$-5923.517 + 122.765451\ T - 25.858\ T \ln(T) + 0.51185E\text{-}3\ T^2 - 3.192767E\text{-}6\ T^3 + 18440\ T^{-1}$ *(100 < T < 250)*

$-3820.135 + 65.443315\ T - 15.961\ T \ln(T) - 18.8702E\text{-}3\ T^2 + 3.121167E\text{-}6\ T^3 - 61960\ T^{-1}$ *(250 < T < 505.078)*

$4559.724 + 4.005269\ T - 8.2590486\ T \ln(T) - 16.814429E\text{-}3\ T^2 + 2.623131E\text{-}6\ T^3 - 1081244\ T^{-1} - 123.07E23\ T^{-9}$ *(505.078 < T < 800)*

$-6221.959 + 138.99688\ T - 28.4512\ T \ln(T) - 123.07E23\ T^{-9}$ *(800 < T < 3000)*

TETRAGONAL_A6

$-2571.517 + 114.503331\,T - 25.858\,T\ln(T) + 0.51185E\text{-}3\,T^2 - 3.192767E\text{-}6\,T^3 + 18440\,T^{-1}$ *(100 < T < 250)*

$-468.135 + 57.181195\,T - 15.961\,T\ln(T) - 18.8702E\text{-}3\,T^2 + 3.121167E\text{-}6\,T^3 - 61960\,T^{-1}$ *(250 < T < 505.078)*

$7911.724 - 4.256851\,T - 8.2590486\,T\ln(T) - 16.814429E\text{-}3\,T^2 + 2.623131E\text{-}6\,T^3 - 1081244\,T^{-1} - 123.07E23\,T^{-9}$ *(505.078 < T < 800)*

$-2869.959 + 130.73476\,T - 28.4512\,T\ln(T) - 123.07E23\,T^{-9}$ *(800 < T < 3000)*

TET_ALPHA1

$-2448.517 + 114.305451\,T - 25.858\,T\ln(T) + 0.51185E\text{-}3\,T^2 - 3.192767E\text{-}6\,T^3 + 18440\,T^{-1}$ *(100 < T < 250)*

$-345.135 + 56.983315\,T - 15.961\,T\ln(T) - 18.8702E\text{-}3\,T^2 + 3.121167E\text{-}6\,T^3 - 61960\,T^{-1}$ *(250 < T < 505.078)*

$8034.724 - 4.454731\,T - 8.2590486\,T\ln(T) - 16.814429E\text{-}3\,T^2 + 2.623131E\text{-}6\,T^3 - 1081244\,T^{-1} - 123.07E23\,T^{-9}$ *(505.078 < T < 800)*

$-2746.959 + 130.53688\,T - 28.4512\,T\ln(T) - 123.07E23\,T^{-9}$ *(800 < T < 3000)*

BCC_A2

$-3558.517 + 116.765451\,T - 25.858\,T\ln(T) + 0.51185E\text{-}3\,T^2 - 3.192767E\text{-}6\,T^3 + 18440\,T^{-1}$ *(100 < T < 250)*

$-1455.135 + 59.443315\,T - 15.961\,T\ln(T) - 18.8702E\text{-}3\,T^2 + 3.121167E\text{-}6\,T^3 - 61960\,T^{-1}$ *(250 < T < 505.078)*

$6924.724 - 1.994731\,T - 8.2590486\,T\ln(T) - 16.814429E\text{-}3\,T^2 + 2.623131E\text{-}6\,T^3 - 1081244\,T^{-1} - 123.07E23\,T^{-9}$ *(505.078 < T < 800)*

$-3856.959 + 132.99688\,T - 28.4512\,T\ln(T) - 123.07E23\,T^{-9}$ *(800 < T < 3000)*

CBCC_A12

$-5958.517 + 122.765451\,T - 25.858\,T\ln(T) + 0.51185E\text{-}3\,T^2 - 3.192767E\text{-}6\,T^3 + 18440\,T^{-1}$ *(100 < T < 250)*

$-3855.135 + 65.443315\,T - 15.961\,T\ln(T) - 18.8702E\text{-}3\,T^2 + 3.121167E\text{-}6\,T^3 - 61960\,T^{-1}$ *(250 < T < 505.078)*

$4524.724 + 4.005269\,T - 8.2590486\,T\ln(T) - 16.814429E\text{-}3\,T^2 + 2.623131E\text{-}6\,T^3 - 1081244\,T^{-1} - 123.07E23\,T^{-9}$ *(505.078 < T < 800)*

$-6256.959 + 138.99688\,T - 28.4512\,T\ln(T) - 123.07E23\,T^{-9}$ *(800 < T < 3000)*

CUB_A13

$-5958.517 + 122.765451\,T - 25.858\,T\ln(T) + 0.51185E\text{-}3\,T^2 - 3.192767E\text{-}6\,T^3 + 18440\,T^{-1}$ *(100 < T < 250)*

$-3855.135 + 65.443315\,T - 15.961\,T\ln(T) - 18.8702E\text{-}3\,T^2 + 3.121167E\text{-}6\,T^3 - 61960\,T^{-1}$ *(250 < T < 505.078)*

$4524.724 + 4.005269\ T - 8.2590486\ T \ln(T) - 16.814429E{-3}\ T^2 + 2.623131E{-6}\ T^3 - 1081244\ T^{-1}$
$- 123.07E23\ T^{-9}$ *(505.078 < T < 800)*
$-6256.959 + 138.99688\ T - 28.4512\ T \ln(T) - 123.07E23\ T^{-9}$ *(800 < T < 3000)*

FCC_A1

$-2448.517 + 114.305451\ T - 25.858\ T \ln(T) + 0.51185E{-3}\ T^2 - 3.192767E{-6}\ T^3 + 18440\ T^{-1}$
(100 < T < 250)
$-345.135 + 56.983315\ T - 15.961\ T \ln(T) - 18.8702E{-3}\ T^2 + 3.121167E{-6}\ T^3 - 61960\ T^{-1}$
(250 < T < 505.078)
$8034.724 - 4.454731\ T - 8.2590486\ T \ln(T) - 16.814429E{-3}\ T^2 + 2.623131E{-6}\ T^3 - 1081244\ T^{-1}$
$- 123.07E23\ T^{-9}$ *(505.078 < T < 800)*
$-2746.959 + 130.53688\ T - 28.4512\ T \ln(T) - 123.07E23\ T^{-9}$ *(800 < T < 3000)*

HCP_A3

$-4058.517 + 115.119451\ T - 25.858\ T \ln(T) + 0.51185E{-3}\ T^2 - 3.192767E{-6}\ T^3 + 18440\ T^{-1}$
(100 < T < 250)
$-1955.135 + 57.797315\ T - 15.961\ T \ln(T) - 18.8702E{-3}\ T^2 + 3.121167E{-6}\ T^3 - 61960\ T^{-1}$
(250 < T < 505.078)
$6424.724 - 3.640731\ T - 8.2590486\ T \ln(T) - 16.814429E{-3}\ T^2 + 2.623131E{-6}\ T^3 - 1081244\ T^{-1}$
$- 123.07E23\ T^{-9}$ *(505.078 < T < 800)*
$-4356.959 + 131.35088\ T - 28.4512\ T \ln(T) - 123.07E23\ T^{-9}$ *(800 < T < 3000)*

HCP_ZN

$-4053.517 + 115.119451\ T - 25.858\ T \ln(T) + 0.51185E{-3}\ T^2 - 3.192767E{-6}\ T^3 + 18440\ T^{-1}$
(100 < T < 250)
$-1950.135 + 57.797315\ T - 15.961\ T \ln(T) - 18.8702E{-3}\ T^2 + 3.121167E{-6}\ T^3 - 61960\ T^{-1}$
(250 < T < 505.078)
$6429.724 - 3.640731\ T - 8.2590486\ T \ln(T) - 16.814429E{-3}\ T^2 + 2.623131E{-6}\ T^3 - 1081244\ T^{-1}$
$- 123.07E23\ T^{-9}$ *(505.078 < T < 800)*
$-4351.959 + 131.35088\ T - 28.4512\ T \ln(T) - 123.07E23\ T^{-9}$ *(800 < T < 3000)*

DHCP

$-4154.997 + 119.305451\ T - 25.858\ T \ln(T) + 0.51185E{-3}\ T^2 - 3.192767E{-6}\ T^3 + 18440\ T^{-1}$
(100 < T < 250)
$-2051.615 + 61.983315\ T - 15.961\ T \ln(T) - 18.8702E{-3}\ T^2 + 3.121167E{-6}\ T^3 - 61960\ T^{-1}$
(250 < T < 505.078)
$6328.244 + 0.545346\ T - 8.2590486\ T \ln(T) - 16.814429E{-3}\ T^2 + 2.623131E{-6}\ T^3 - 1081244\ T^{-1}$
$- 123.07E23\ T^{-9}$ *(505.078 < T < 800)*
$-4453.439 + 135.536959\ T - 28.4512\ T \ln(T) - 123.07E23\ T^{-9}$ *(800 < T < 3000)*

Data relative to BCT_A5

DIAMOND_A4

$-1621.091 - 8.757666\ T + 2.886\ T \ln(T) - 8.6516E\text{-}3\ T^2 + 5.921567E\text{-}6\ T^3 + 7175\ T^{-1}$ *(100 < T < 250)*
$-3724.473 + 48.56447\ T - 7.011\ T \ln(T) + 10.73045E\text{-}3\ T^2 - 0.392367E\text{-}6\ T^3 + 87575\ T^{-1}$ *(250 < T < 298.15)*
$-3207.866 + 39.403225\ T - 5.6140771\ T \ln(T) + 10.294918E\text{-}3\ T^2 - 1.33672E\text{-}6\ T^3 + 59416\ T^{-1}$ *(298.15 < T < 505.078)*
$-11587.725 + 100.841271\ T - 13.3160285\ T \ln(T) + 8.239147E\text{-}3\ T^2 - 0.838684E\text{-}6\ T^3 + 1078700\ T^{-1} + 123.07E23\ T^{-9}$ *(505.078 < T < 800)*
$-2652.392 + 8.399655\ T + 123.07E23\ T^{-9}$ *(800 < T < 3000)*

LIQUID

$7103.092 - 14.087767\ T + 147.031E\text{-}20\ T^7$ *(100 < T < 505.078)*
$6971.586 - 13.814383\ T + 123.07E23\ T^{-9}$ *(505.078 < T < 3000)*

RHOMBOHEDRAL_A7

2035 *(100 < T < 3000)*

TETRAGONAL_A6

5387 - 8.26212 T *(100 < T < 3000)*

TET_ALPHA1

5510 - 8.46 T *(100 < T < 3000)*

BCC_A2

4400 - 6 T *(100 < T < 3000)*

CBCC_A12

2000 *(100 < T < 3000)*

CUB_A13

2000 *(100 < T < 3000)*

FCC_A1

5510 - 8.46 T *(100 < T < 3000)*

HCP_A3

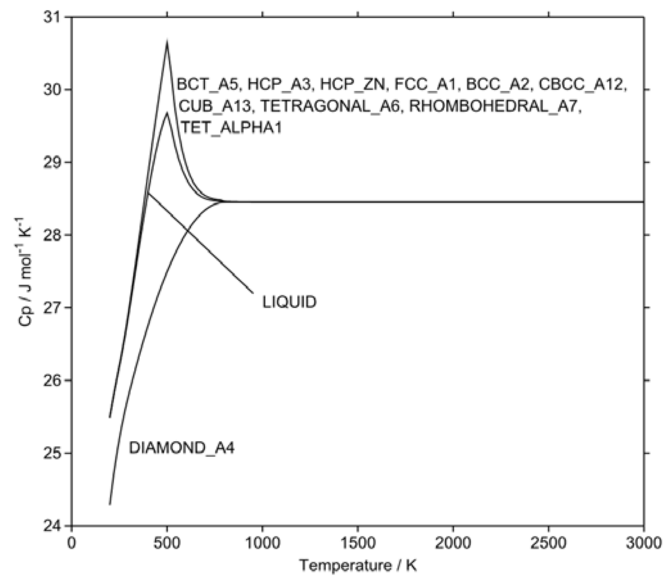
3900 - 7.646 T *(100 < T < 3000)*

HCP_ZN

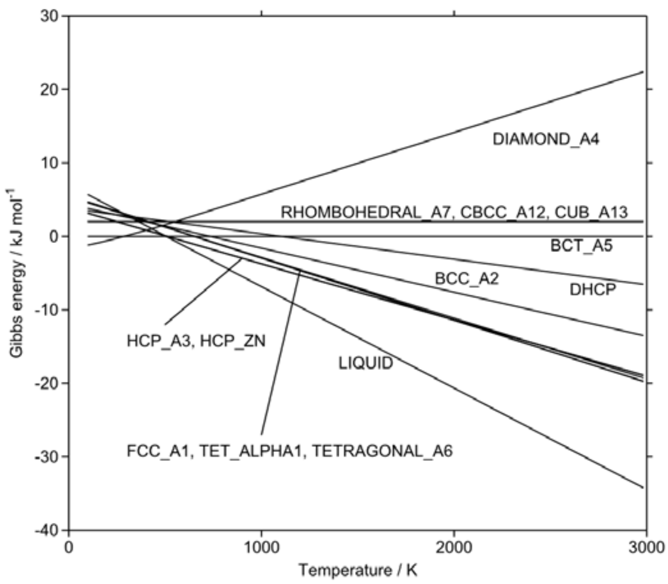
3905 - 7.646 T *(100 < T < 3000)*

DHCP

3803.52 - 3.46 T *(100 < T < 3000)*



Heat capacity of Sn



Gibbs energy of phases of Sn relative to BCT_A5

Sr

Source of data: *JANAF [FCC_A1, BCC_A2, LIQUID]*
Saunders et al. [HCP_A3]

BCC_A2

-6779.234 + 116.583654 T - 25.6708365 T ln(T) - 3.126762E-3 T^2 + 0.22965E-6 T^3 + 27649 T^{-1} *(298.15 < T < 820)*

-6970.594 + 122.067301 T - 26.57 T ln(T) - 1.9493E-3 T^2 - 0.017895E-6 T^3 + 16495 T^{-1} *(820 < T < 1050)*

8168.357 + 0.423037 T - 9.7788593 T ln(T) - 9.539908E-3 T^2 + 0.520221E-6 T^3 - 2414794 T^{-1} *(1050 < T < 3000)*

FCC_A1

$-7532.367 + 107.183879\,T - 23.905\,T\ln(T) - 4.61225E\text{-}3\,T^2 - 0.167477E\text{-}6\,T^3 - 2055\,T^{-1}$

(298.15 < T < 820)

$-13380.102 + 153.196104\,T - 30.0905432\,T\ln(T) - 3.251266E\text{-}3\,T^2 + 0.184189E\text{-}6\,T^3 + 850134\,T^{-1}$

(820 < T < 3000)

LIQUID

$2194.997 - 10.118994\,T - 5.0668978\,T\ln(T) - 31.840595E\text{-}3\,T^2 + 4.981237E\text{-}6\,T^3 - 265559\,T^{-1}$

(298.15 < T < 1050)

$-10855.29 + 213.406219\,T - 39.463\,T\ln(T)$ *(1050 < T < 3000)*

HCP_A3

$-7282.367 + 107.883879\,T - 23.905\,T\ln(T) - 4.61225E\text{-}3\,T^2 - 0.167477E\text{-}6\,T^3 - 2055\,T^{-1}$

(298.15 < T < 820)

$-13130.102 + 153.896104\,T - 30.0905432\,T\ln(T) - 3.251266E\text{-}3\,T^2 + 0.184189E\text{-}6\,T^3 + 850134\,T^{-1}$

(820 < T < 3000)

Data relative to FCC_A1

BCC_A2

$753.133 + 9.399775\,T - 1.7658365\,T\ln(T) + 1.485488E\text{-}3\,T^2 + 0.397127E\text{-}6\,T^3 + 29704\,T^{-1}$

(298.15 < T < 820)

$6409.508 - 31.128803\,T + 3.5205432\,T\ln(T) + 1.301966E\text{-}3\,T^2 - 0.202084E\text{-}6\,T^3 - 833639\,T^{-1}$

(820 < T < 1050)

$21548.459 - 152.773067\,T + 20.3116839\,T\ln(T) - 6.288642E\text{-}3\,T^2 + 0.336032E\text{-}6\,T^3 - 3264928\,T^{-1}$

(1050 < T < 3000)

LIQUID

$9727.364 - 117.302873\,T + 18.8381022\,T\ln(T) - 27.228345E\text{-}3\,T^2 + 5.148714E\text{-}6\,T^3 - 263504\,T^{-1}$

(298.15 < T < 820)

$15575.099 - 163.315098\,T + 25.0236454\,T\ln(T) - 28.589329E\text{-}3\,T^2 + 4.797048E\text{-}6\,T^3 - 1115693\,T^{-1}$

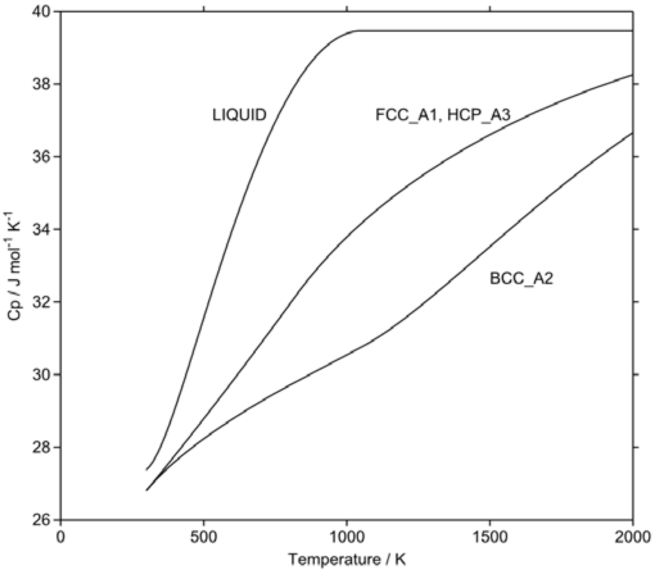
(820 < T < 1050)

$2524.812 + 60.210115\,T - 9.3724568\,T\ln(T) + 3.251266E\text{-}3\,T^2 - 0.184189E\text{-}6\,T^3 - 850134\,T^{-1}$

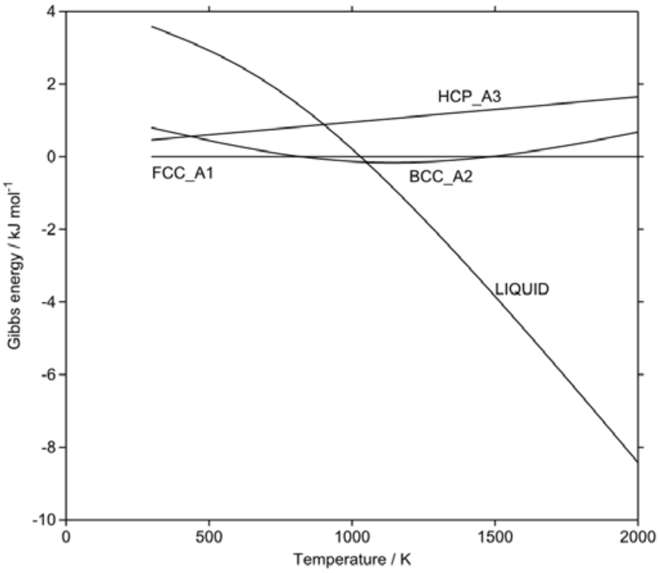
(1050 < T < 3000)

HCP_A3

$250 + 0.7\,T$ *(298.15 < T < 3000)*



Heat capacity of Sr



Gibbs energy of phases of Sr relative to FCC_A1

Ta

Source of data: *JANAF [BCC_A2, LIQUID]*
A Fernandez Guillermet, W Huang, Z. Metallkde., 1988, ***79****, 88 [FCC_A1, HCP_A3]*

BCC_A2

$-7285.889 + 119.139857\,T - 23.7592624\,T\ln(T) - 2.623033E\text{-}3\,T^2 + 0.170109E\text{-}6\,T^3 - 3293\,T^{-1}$
$(298.15 < T < 1300)$

$-22389.955 + 243.88676\,T - 41.137088\,T\ln(T) + 6.167572E\text{-}3\,T^2 - 0.655136E\text{-}6\,T^3 + 2429586\,T^{-1}$
$(1300 < T < 2500)$

$229382.886 - 722.59722\,T + 78.5244752\,T\ln(T) - 17.983376E\text{-}3\,T^2 + 0.195033E\text{-}6\,T^3 - 93813648\,T^{-1}$
$(2500 < T < 3290)$

$-1042384.014 + 2985.491246\,T - 362.1591318\,T\ln(T) + 43.117795E\text{-}3\,T^2 - 1.055148E\text{-}6\,T^3$
$+ 554714342\,T^{-1}$ $(3290 < T < 6000)$

LIQUID

$21875.086 + 111.561128\,T - 23.7592624\,T\ln(T) - 2.623033E\text{-}3\,T^2 + 0.170109E\text{-}6\,T^3 - 3293\,T^{-1}$
$(298.15 < T < 1000)$

$43884.339 - 61.981795\,T + 0.0279523\,T\ln(T) - 12.330066E\text{-}3\,T^2 + 0.614599E\text{-}6\,T^3 - 3523338\,T^{-1}$
$(1000 < T < 3290)$

$-6314.543 + 258.110873\,T - 41.84\,T\ln(T)$ $(3290 < T < 6000)$

FCC_A1

$8714.111 + 120.839857\,T - 23.7592624\,T\ln(T) - 2.623033E\text{-}3\,T^2 + 0.170109E\text{-}6\,T^3 - 3293\,T^{-1}$
$(298.15 < T < 1300)$

$-6389.955 + 245.58676\ T - 41.137088\ T\ln(T) + 6.167572E\text{-}3\ T^2 - 0.655136E\text{-}6\ T^3 + 2429586\ T^{-1}$ *(1300 < T < 2500)*

$245382.886 - 720.89722\ T + 78.5244752\ T\ln(T) - 17.983376E\text{-}3\ T^2 + 0.195033E\text{-}6\ T^3 - 93813648\ T^{-1}$ *(2500 < T < 3290)*

$-1026384.014 + 2987.191246\ T - 362.1591318\ T\ln(T) + 43.117795E\text{-}3\ T^2 - 1.055148E\text{-}6\ T^3 + 554714342\ T^{-1}$ *(3290 < T < 6000)*

HCP_A3

$4714.111 + 121.539857\ T - 23.7592624\ T\ln(T) - 2.623033E\text{-}3\ T^2 + 0.170109E\text{-}6\ T^3 - 3293\ T^{-1}$ *(298.15 < T < 1300)*

$-10389.955 + 246.28676\ T - 41.137088\ T\ln(T) + 6.167572E\text{-}3\ T^2 - 0.655136E\text{-}6\ T^3 + 2429586\ T^{-1}$ *(1300 < T < 2500)*

$241382.886 - 720.19722\ T + 78.5244752\ T\ln(T) - 17.983376E\text{-}3\ T^2 + 0.195033E\text{-}6\ T^3 - 93813648\ T^{-1}$ *(2500 < T < 3290)*

$-1030384.014 + 2987.891246\ T - 362.1591318\ T\ln(T) + 43.117795E\text{-}3\ T^2 - 1.055148E\text{-}6\ T^3 + 554714342\ T^{-1}$ *(3290 < T < 6000)*

Data relative to BCC_A2

LIQUID

$29160.975 - 7.578729\ T$ *(298.15 < T < 1000)*

$51170.228 - 181.121652\ T + 23.7872147\ T\ln(T) - 9.707033E\text{-}3\ T^2 + 0.44449E\text{-}6\ T^3 - 3520045\ T^{-1}$ *(1000 < T < 1300)*

$66274.294 - 305.868555\ T + 41.1650403\ T\ln(T) - 18.497638E\text{-}3\ T^2 + 1.269735E\text{-}6\ T^3 - 5952924\ T^{-1}$ *(1300 < T < 2500)*

$-185498.547 + 660.615425\ T - 78.4965229\ T\ln(T) + 5.65331E\text{-}3\ T^2 + 0.419566E\text{-}6\ T^3 + 90290310\ T^{-1}$ *(2500 < T < 3290)*

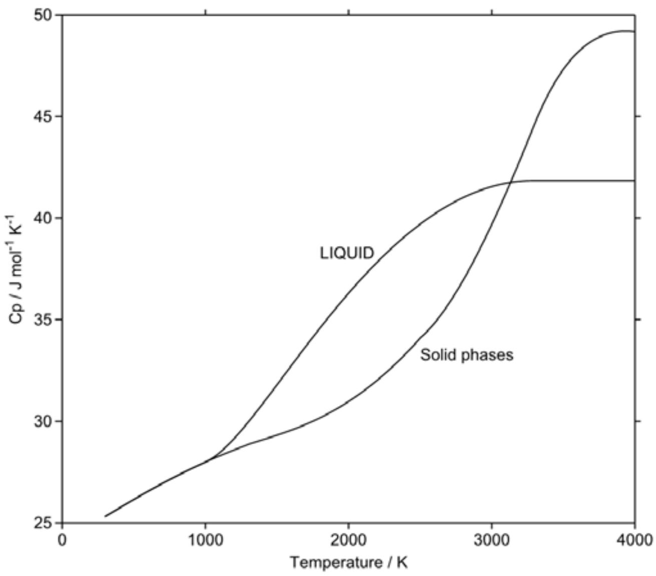
$1036069.471 - 2727.380373\ T + 320.3191318\ T\ln(T) - 43.117795E\text{-}3\ T^2 + 1.055148E\text{-}6\ T^3 - 554714342\ T^{-1}$ *(3290 < T < 6000)*

FCC_A1

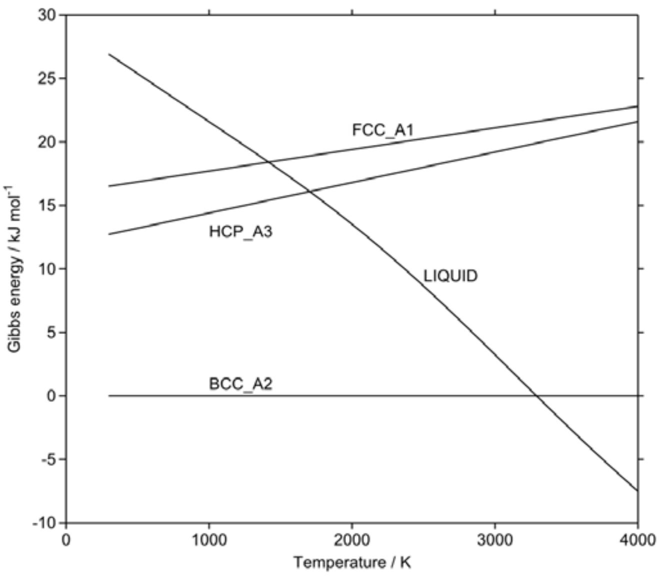
$16000 + 1.7\ T$ *(298.15 < T < 6000)*

HCP_A3

$12000 + 2.4\ T$ *(298.15 < T < 6000)*



Heat capacity of Ta



Gibbs energy of phases of Ta relative to BCC_A2

Tb

Source of data: *Hultgren, modified by M H Rand*

HCP_A3

$-20842.158 + 409.309555\ T - 77.5006\ T \ln(T) + 83.2265E{-3}\ T^2 - 25.672833E{-6}\ T^3 + 562430\ T^{-1}$ *(298.15 < T < 600)*

$-8772.606 + 102.61162\ T - 25.8659\ T \ln(T) - 2.757005E{-3}\ T^2 - 0.805838E{-6}\ T^3 + 172355\ T^{-1}$ *(600 < T < 1200)*

$-7944.942 + 101.7776\ T - 25.9584\ T \ln(T) - 1.676335E{-3}\ T^2 - 1.067632E{-6}\ T^3$ *(1200 < T < 1562)*

$-265240.309 + 1456.042685\ T - 200.2156949\ T \ln(T) + 41.615159E{-3}\ T^2 - 2.044697E{-6}\ T^3 + 65043790\ T^{-1}$ *(1562 < T < 3000)*

BCC_A2

$-16674.323 + 406.656848\ T - 77.5006\ T \ln(T) + 83.2265E{-3}\ T^2 - 25.672833E{-6}\ T^3 + 562430\ T^{-1}$ *(298.15 < T < 600)*

$-4604.771 + 99.958913\ T - 25.8659\ T \ln(T) - 2.757005E{-3}\ T^2 - 0.805838E{-6}\ T^3 + 172355\ T^{-1}$ *(600 < T < 1200)*

$633060.245 - 5157.777795\ T + 706.5805957\ T \ln(T) - 373.763517E{-3}\ T^2 + 34.100235E{-6}\ T^3 - 103233571\ T^{-1}$ *(1200 < T < 1562)*

$-23398.029 + 257.388486\ T - 46.4842\ T \ln(T)$ *(1562 < T < 3000)*

LIQUID

$3945.831 + 29.867521\ T - 14.252646\ T \ln(T) - 20.466105E{-3}\ T^2 + 2.17475E{-6}\ T^3 - 160724\ T^{-1}$ *(298.15 < T < 1562)*

$-13247.649 + 251.16889\ T - 46.4842\ T \ln(T)$ *(1562 < T < 3000)*

Data relative to HCP_A3

BCC_A2

$4167.835 - 2.652707\ T$ *(298.15 < T < 1200)*

$641005.187 - 5259.555395\ T + 732.5389957\ T\ \ln(T) - 372.087182E\text{-}3\ T^2 + 35.167867E\text{-}6\ T^3 - 103233571\ T^{-1}$ *(1200 < T < 1562)*

$241842.28 - 1198.654199\ T + 153.7314949\ T\ \ln(T) - 41.615159E\text{-}3\ T^2 + 2.044697E\text{-}6\ T^3 - 65043790\ T^{-1}$ *(1562 < T < 3000)*

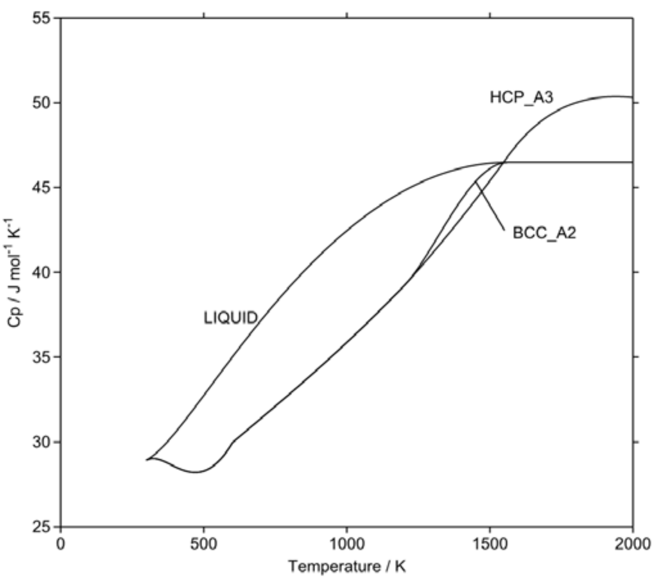
LIQUID

$24787.989 - 379.442034\ T + 63.247954\ T\ \ln(T) - 103.692605E\text{-}3\ T^2 + 27.847583E\text{-}6\ T^3 - 723154\ T^{-1}$ *(298.15 < T < 600)*

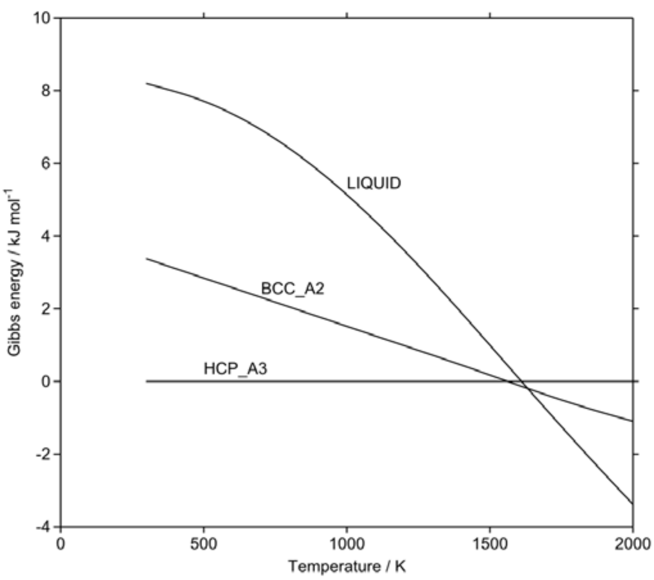
$12718.437 - 72.744099\ T + 11.613254\ T\ \ln(T) - 17.7091E\text{-}3\ T^2 + 2.980588E\text{-}6\ T^3 - 333079\ T^{-1}$ *(600 < T < 1200)*

$11890.773 - 71.910079\ T + 11.705754\ T\ \ln(T) - 18.78977E\text{-}3\ T^2 + 3.242382E\text{-}6\ T^3 - 160724\ T^{-1}$ *(1200 < T < 1562)*

$251992.66 - 1204.873795\ T + 153.7314949\ T\ \ln(T) - 41.615159E\text{-}3\ T^2 + 2.044697E\text{-}6\ T^3 - 65043790\ T^{-1}$ *(1562 < T < 3000)*



Heat capacity of Tb



Gibbs energy of phases of Tb relative to HCP_A3

Tc

Source of data: *A Fernandez Guillermet, G Grimvall, J. Less Common Metals, 1989, **147**, 195 [HCP_A3, LIQUID]*
Saunders et al. [FCC_A1, BCC_A2]

HCP_A3

$-7947.794 + 132.5101\ T - 24.3394\ T\ \ln(T) - 2.954747E\text{-}3\ T^{2} + 63855\ T^{-1}$ *(298.15 < T < 2430)*
$-47759.99 + 318.286\ T - 47\ T\ \ln(T) + 663.829E30\ T^{-9}$ *(2430 < T < 4000)*

LIQUID

$22454.34 + 120.1971\ T - 24.3394\ T\ \ln(T) - 2.954747E\text{-}3\ T^{2} + 63855\ T^{-1} - 962.385E\text{-}24\ T^{7}$
(298.15 < T < 2430)
$-12221.9 + 303.7538\ T - 47\ T\ \ln(T)$ *(2430 < T < 4000)*

BCC_A2

$10052.206 + 128.0101\ T - 24.3394\ T\ \ln(T) - 2.954747E\text{-}3\ T^{2} + 63855\ T^{-1}$ *(298.15 < T < 2430)*
$-29759.99 + 313.786\ T - 47\ T\ \ln(T) + 663.829E30\ T^{-9}$ *(2430 < T < 4000)*

FCC_A1

$2052.206 + 131.0101\ T - 24.3394\ T\ \ln(T) - 2.954747E\text{-}3\ T^{2} + 63855\ T^{-1}$ *(298.15 < T < 2430)*
$-37759.99 + 316.786\ T - 47\ T\ \ln(T) + 663.829E30\ T^{-9}$ *(2430 < T < 4000)*

Data relative to HCP_A3

LIQUID

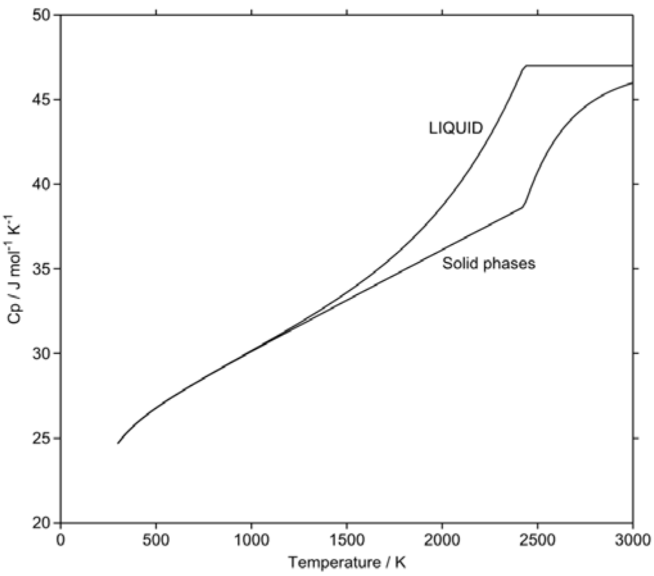
$30402.134 - 12.313\ T - 962.385E\text{-}24\ T^{7}$ *(298.15 < T < 2430)*
$35538.09 - 14.5322\ T - 663.829E30\ T^{-9}$ *(2430 < T < 4000)*

BCC_A2

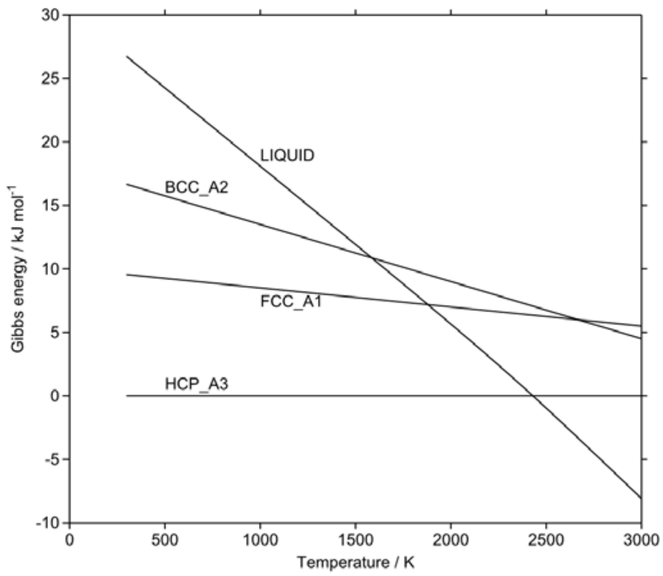
$18000 - 4.5\ T$ *(298.15 < T < 4000)*

FCC_A1

$10000 - 1.5\ T$ *(298.15 < T < 4000)*



Heat capacity of Tc



Gibbs energy of phases of Tc relative to HCP_A3

Te

Source of data: *Based on data from A Davydov, M H Rand and B B Argent, CALPHAD, 1995, 19(3), 375 [HEXAGONAL_A8, LIQUID]*

HEXAGONAL_A8

$-10544.679 + 183.372894\ T - 35.6687\ T\ln(T) + 15.83435E{-3}\ T^2 - 5.240417E{-6}\ T^3 + 155015\ T^{-1}$ *(298.15 < T < 722.66)*

$9160.595 - 129.265373\ T + 13.004\ T\ln(T) - 36.2361E{-3}\ T^2 + 5.006367E{-6}\ T^3 - 1286810\ T^{-1}$ *(722.66 < T < 1150)*

$-12781.349 + 174.901226\ T - 32.5596\ T\ln(T)$ *(1150 < T < 1600)*

LIQUID

$-17554.731 + 685.877639\ T - 126.318\ T\ln(T) + 221.9435E{-3}\ T^2 - 94.2075E{-6}\ T^3 + 827930\ T^{-1}$ *(298.15 < T < 626.49)*

$-3165763.484 + 46756.357035\ T - 7196.41\ T\ln(T) + 7097.75E{-3}\ T^2 - 1306.928333E{-6}\ T^3 + 258051000\ T^{-1}$ *(626.49 < T < 722.66)*

$180326.959 - 1500.579094\ T + 202.743\ T\ln(T) - 142.016E{-3}\ T^2 + 16.129733E{-6}\ T^3 - 24238450\ T^{-1}$ *(722.66 < T < 1150)*

$6328.687 + 148.708299\ T - 32.5596\ T\ln(T)$ *(1150 < T < 1600)*

Data relative to HEXAGONAL_A8

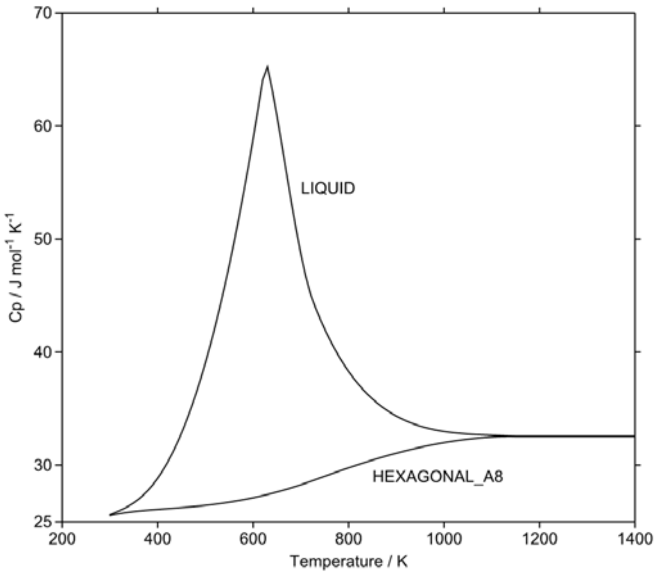
LIQUID

$-7010.052 + 502.504745\ T - 90.6493\ T\ln(T) + 206.10915E{-3}\ T^2 - 88.967083E{-6}\ T^3 + 672915\ T^{-1}$ *(298.15 < T < 626.49)*

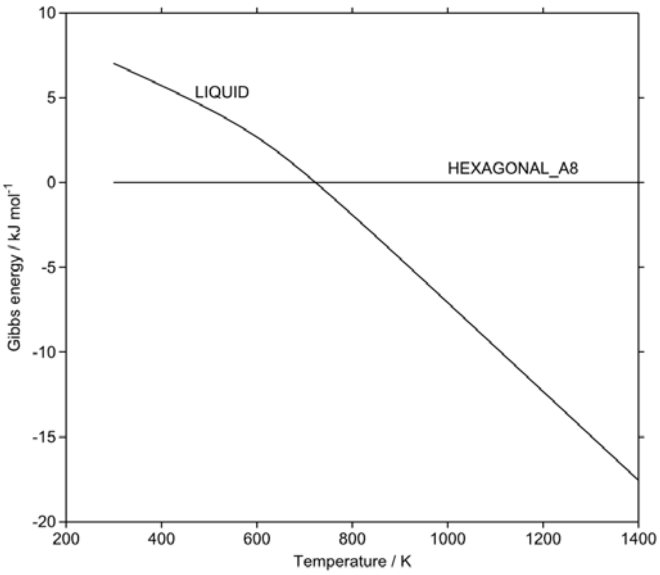
$-3155218.805 + 46572.984141\ T - 7160.7413\ T \ln(T) + 7081.91565E\text{-}3\ T^2 - 1301.687916E\text{-}6\ T^3$
$+ 257895985\ T^{-1}$ *(626.49 < T < 722.66)*

$171166.364 - 1371.313721\ T + 189.739\ T \ln(T) - 105.7799E\text{-}3\ T^2 + 11.123366E\text{-}6\ T^3 - 22951640\ T^{-1}$
(722.66 < T < 1150)

$19110.036 - 26.192927\ T$ *(1150 < T < 1600)*



Heat capacity of Te



Gibbs energy of phases of Te relative to HEXAGONAL_A8

Th

Source of data: *M H Rand (Unpublished work), modified by A T Dinsdale (2002)*

FCC_A1

$-7732.08 + 116.273975\ T - 24.841\ T \ln(T) - 2.36725E\text{-}3\ T^2 - 0.52883E\text{-}6\ T^3 + 13010\ T^{-1}$
(298.15 < T < 1633)

$-37352.871 + 236.906118\ T - 39.107\ T \ln(T) - 3.58025E\text{-}3\ T^2 + 0.236893E\text{-}6\ T^3 + 7981000\ T^{-1}$
(1633 < T < 2900)

$-33353.313 + 283.231045\ T - 46.024\ T \ln(T)$ *(2900 < T < 4000)*

BCC_A2

$-2321.06 + 133.531195\ T - 28.244\ T \ln(T) + 0.43775E\text{-}3\ T^2 - 0.53048E\text{-}6\ T^3 + 91190\ T^{-1}$
(298.15 < T < 1633)

$-115978.348 + 800.909049\ T - 116.453\ T \ln(T) + 30.98E\text{-}3\ T^2 - 2.536883E\text{-}6\ T^3 + 27512600\ T^{-1}$
(1633 < T < 2023)

$-33602.796 + 208.774709\ T - 35.813\ T \ln(T) - 3.46655E\text{-}3\ T^2 + 0.166067E\text{-}6\ T^3 + 11876950\ T^{-1}$
(2023 < T < 3600)

$-34333.615 + 283.181494\ T - 46.024\ T \ln(T)$ *(3600 < T < 4000)*

LIQUID

$5031.109 + 110.886346\,T - 24.987\,T\ln(T) - 1.68345E\text{-}3\,T^2 - 0.909067E\text{-}6\,T^3 + 10865\,T^{-1}$ *(298.15 < T < 1499.8)*

$-15602.847 + 127.657716\,T - 24.03\,T\ln(T) - 13.6421E\text{-}3\,T^2 + 1.210117E\text{-}6\,T^3 + 7111100\,T^{-1}$ *(1499.8 < T < 2014.5)*

$-17273.382 + 275.001274\,T - 46.024\,T\ln(T)$ *(2014.5 < T < 4000)*

Data relative to FCC_A1

BCC_A2

$5411.02 + 17.25722\,T - 3.403\,T\ln(T) + 2.805E\text{-}3\,T^2 - 0.00165E\text{-}6\,T^3 + 78180\,T^{-1}$ *(298.15 < T < 1633)*

$-78625.477 + 564.002931\,T - 77.346\,T\ln(T) + 34.56025E\text{-}3\,T^2 - 2.773776E\text{-}6\,T^3 + 19531600\,T^{-1}$ *(1633 < T < 2023)*

$3750.075 - 28.131409\,T + 3.294\,T\ln(T) + 0.1137E\text{-}3\,T^2 - 0.070826E\text{-}6\,T^3 + 3895950\,T^{-1}$ *(2023 < T < 2900)*

$-249.483 - 74.456336\,T + 10.211\,T\ln(T) - 3.46655E\text{-}3\,T^2 + 0.166067E\text{-}6\,T^3 + 11876950\,T^{-1}$ *(2900 < T < 3600)*

$-980.302 - 0.049551\,T$ *(3600 < T < 4000)*

LIQUID

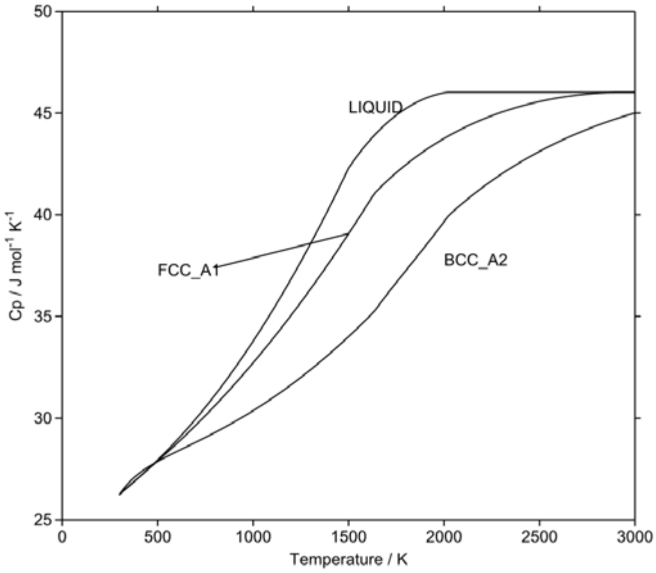
$12763.189 - 5.387629\,T - 0.146\,T\ln(T) + 0.6838E\text{-}3\,T^2 - 0.380237E\text{-}6\,T^3 - 2145\,T^{-1}$ *(298.15 < T < 1499.8)*

$-7870.767 + 11.383741\,T + 0.811\,T\ln(T) - 11.27485E\text{-}3\,T^2 + 1.738947E\text{-}6\,T^3 + 7098090\,T^{-1}$ *(1499.8 < T < 1633)*

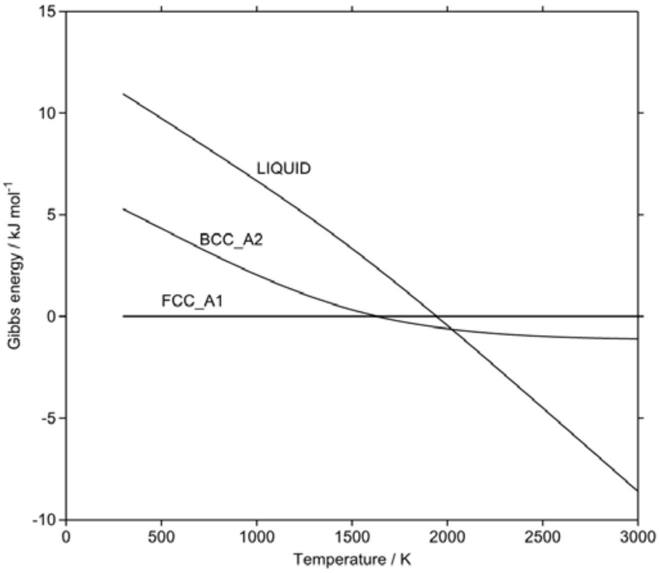
$21750.024 - 109.248402\,T + 15.077\,T\ln(T) - 10.06185E\text{-}3\,T^2 + 0.973224E\text{-}6\,T^3 - 869900\,T^{-1}$ *(1633 < T < 2014.5)*

$20079.489 + 38.095156\,T - 6.917\,T\ln(T) + 3.58025E\text{-}3\,T^2 - 0.236893E\text{-}6\,T^3 - 7981000\,T^{-1}$ *(2014.5 < T < 2900)*

$16079.931 - 8.229771\,T$ *(2900 < T < 4000)*



Heat capacity of Th



Gibbs energy of phases of Th relative to FCC_A1

Ti

Source of data: *A T Dinsdale (Unpublished work) [HCP_A3, BCC_A2, LIQUID]*
Saunders et al. [FCC_A1]
Kaufman [BCC_A12, CUB_A13]
M Pajunen (Unpublished work) [DIAMOND_A4]
COST507 database [BCT_A5]

HCP_A3

$-8059.921 + 133.615208\ T - 23.9933\ T\ln(T) - 4.777975E\text{-}3\ T^2 + 0.106716E\text{-}6\ T^3 + 72636\ T^{-1}$
(298.15 < T < 900)
$-7811.815 + 132.988068\ T - 23.9887\ T\ln(T) - 4.2033E\text{-}3\ T^2 - 0.090876E\text{-}6\ T^3 + 42680\ T^{-1}$
(900 < T < 1155)
$908.837 + 66.976538\ T - 14.9466\ T\ln(T) - 8.1465E\text{-}3\ T^2 + 0.202715E\text{-}6\ T^3 - 1477660\ T^{-1}$
(1155 < T < 1941)
$-124526.786 + 638.806871\ T - 87.2182461\ T\ln(T) + 8.204849E\text{-}3\ T^2 - 0.304747E\text{-}6\ T^3 + 36699805\ T^{-1}$
(1941 < T < 4000)

BCC_A2

$-1272.064 + 134.71418\ T - 25.5768\ T\ln(T) - 0.663845E\text{-}3\ T^2 - 0.278803E\text{-}6\ T^3 + 7208\ T^{-1}$
(298.15 < T < 1155)
$6667.385 + 105.366379\ T - 22.3771\ T\ln(T) + 1.21707E\text{-}3\ T^2 - 0.84534E\text{-}6\ T^3 - 2002750\ T^{-1}$
(1155 < T < 1941)
$26483.26 - 182.426471\ T + 19.0900905\ T\ln(T) - 22.00832E\text{-}3\ T^2 + 1.228863E\text{-}6\ T^3 + 1400501\ T^{-1}$
(1941 < T < 4000)

LIQUID

$4134.494 + 126.63427\ T - 23.9933\ T \ln(T) - 4.777975E\text{-}3\ T^2 + 0.106716E\text{-}6\ T^3 + 72636\ T^{-1}$
(298.15 < T < 900)
$4382.601 + 126.00713\ T - 23.9887\ T \ln(T) - 4.2033E\text{-}3\ T^2 - 0.090876E\text{-}6\ T^3 + 42680\ T^{-1}$
(900 < T < 1155)
$13103.253 + 59.9956\ T - 14.9466\ T \ln(T) - 8.1465E\text{-}3\ T^2 + 0.202715E\text{-}6\ T^3 - 1477660\ T^{-1}$
(1155 < T < 1300)
$369519.198 - 2554.0225\ T + 342.059267\ T \ln(T) - 163.409355E\text{-}3\ T^2 + 12.457117E\text{-}6\ T^3 - 67034516\ T^{-1}$
(1300 < T < 1941)
$-19887.066 + 298.7367\ T - 46.29\ T \ln(T)$ *(1941 < T < 4000)*

BCT_A5

$-3457.721 + 133.615208\ T - 23.9933\ T \ln(T) - 4.777975E\text{-}3\ T^2 + 0.106716E\text{-}6\ T^3 + 72636\ T^{-1}$
(298.15 < T < 900)
$-3209.615 + 132.988068\ T - 23.9887\ T \ln(T) - 4.2033E\text{-}3\ T^2 - 0.090876E\text{-}6\ T^3 + 42680\ T^{-1}$
(900 < T < 1155)
$5511.037 + 66.976538\ T - 14.9466\ T \ln(T) - 8.1465E\text{-}3\ T^2 + 0.202715E\text{-}6\ T^3 - 1477660\ T^{-1}$
(1155 < T < 1941)
$-119924.586 + 638.806871\ T - 87.2182461\ T \ln(T) + 8.204849E\text{-}3\ T^2 - 0.304747E\text{-}6\ T^3 + 36699805\ T^{-1}$
(1941 < T < 3000)

DIAMOND_A4

$16940.079 + 133.615208\ T - 23.9933\ T \ln(T) - 4.777975E\text{-}3\ T^2 + 0.106716E\text{-}6\ T^3 + 72636\ T^{-1}$
(298.15 < T < 900)
$17188.185 + 132.988068\ T - 23.9887\ T \ln(T) - 4.2033E\text{-}3\ T^2 - 0.090876E\text{-}6\ T^3 + 42680\ T^{-1}$
(900 < T < 1155)
$25908.837 + 66.976538\ T - 14.9466\ T \ln(T) - 8.1465E\text{-}3\ T^2 + 0.202715E\text{-}6\ T^3 - 1477660\ T^{-1}$
(1155 < T < 1941)
$-99526.786 + 638.806871\ T - 87.2182461\ T \ln(T) + 8.204849E\text{-}3\ T^2 - 0.304747E\text{-}6\ T^3 + 36699805\ T^{-1}$
(1941 < T < 4000)

CBCC_A12

$-3457.721 + 133.615208\ T - 23.9933\ T \ln(T) - 4.777975E\text{-}3\ T^2 + 0.106716E\text{-}6\ T^3 + 72636\ T^{-1}$
(298.15 < T < 900)
$-3209.615 + 132.988068\ T - 23.9887\ T \ln(T) - 4.2033E\text{-}3\ T^2 - 0.090876E\text{-}6\ T^3 + 42680\ T^{-1}$
(900 < T < 1155)
$5511.037 + 66.976538\ T - 14.9466\ T \ln(T) - 8.1465E\text{-}3\ T^2 + 0.202715E\text{-}6\ T^3 - 1477660\ T^{-1}$
(1155 < T < 1941)
$-119924.586 + 638.806871\ T - 87.2182461\ T \ln(T) + 8.204849E\text{-}3\ T^2 - 0.304747E\text{-}6\ T^3 + 36699805\ T^{-1}$
(1941 < T < 4000)

CUB_A13

$-528.721 + 133.615208\ T - 23.9933\ T \ln(T) - 4.777975E\text{-}3\ T^2 + 0.106716E\text{-}6\ T^3 + 72636\ T^{-1}$
(298.15 < T < 900)
$-280.615 + 132.988068\ T - 23.9887\ T \ln(T) - 4.2033E\text{-}3\ T^2 - 0.090876E\text{-}6\ T^3 + 42680\ T^{-1}$
(900 < T < 1155)
$8440.037 + 66.976538\ T - 14.9466\ T \ln(T) - 8.1465E\text{-}3\ T^2 + 0.202715E\text{-}6\ T^3 - 1477660\ T^{-1}$
(1155 < T < 1941)
$-116995.586 + 638.806871\ T - 87.2182461\ T \ln(T) + 8.204849E\text{-}3\ T^2 - 0.304747E\text{-}6\ T^3 + 36699805\ T^{-1}$
(1941 < T < 4000)

FCC_A1

$-2059.921 + 133.515208\ T - 23.9933\ T \ln(T) - 4.777975E\text{-}3\ T^2 + 0.106716E\text{-}6\ T^3 + 72636\ T^{-1}$
(298.15 < T < 900)
$-1811.815 + 132.888068\ T - 23.9887\ T \ln(T) - 4.2033E\text{-}3\ T^2 - 0.090876E\text{-}6\ T^3 + 42680\ T^{-1}$
(900 < T < 1155)
$6908.837 + 66.876538\ T - 14.9466\ T \ln(T) - 8.1465E\text{-}3\ T^2 + 0.202715E\text{-}6\ T^3 - 1477660\ T^{-1}$
(1155 < T < 1941)
$-118526.786 + 638.706871\ T - 87.2182461\ T \ln(T) + 8.204849E\text{-}3\ T^2 - 0.304747E\text{-}6\ T^3 + 36699805\ T^{-1}$
(1941 < T < 4000)

Data relative to HCP_A3

BCC_A2

$6787.857 + 1.098972\ T - 1.5835\ T \ln(T) + 4.11413E\text{-}3\ T^2 - 0.385519E\text{-}6\ T^3 - 65428\ T^{-1}$
(298.15 < T < 900)
$6539.751 + 1.726112\ T - 1.5881\ T \ln(T) + 3.539455E\text{-}3\ T^2 - 0.187927E\text{-}6\ T^3 - 35472\ T^{-1}$
(900 < T < 1155)
$5758.548 + 38.389841\ T - 7.4305\ T \ln(T) + 9.36357E\text{-}3\ T^2 - 1.048055E\text{-}6\ T^3 - 525090\ T^{-1}$
(1155 < T < 1941)
$151010.046 - 821.233342\ T + 106.3083366\ T \ln(T) - 30.213169E\text{-}3\ T^2 + 1.53361E\text{-}6\ T^3 - 35299304\ T^{-1}$
(1941 < T < 4000)

LIQUID

$12194.415 - 6.980938\ T$ *(298.15 < T < 1300)*
$368610.361 - 2620.999038\ T + 357.005867\ T \ln(T) - 155.262855E\text{-}3\ T^2 + 12.254402E\text{-}6\ T^3$
$- 65556856\ T^{-1}$ *(1300 < T < 1941)*
$104639.72 - 340.070171\ T + 40.9282461\ T \ln(T) - 8.204849E\text{-}3\ T^2 + 0.304747E\text{-}6\ T^3 - 36699805\ T^{-1}$
(1941 < T < 4000)

BCT_A5

4602.2 *(298.15 < T < 3000)*

DIAMOND_A4

25000 *(298.15 < T < 4000)*

CBCC_A12

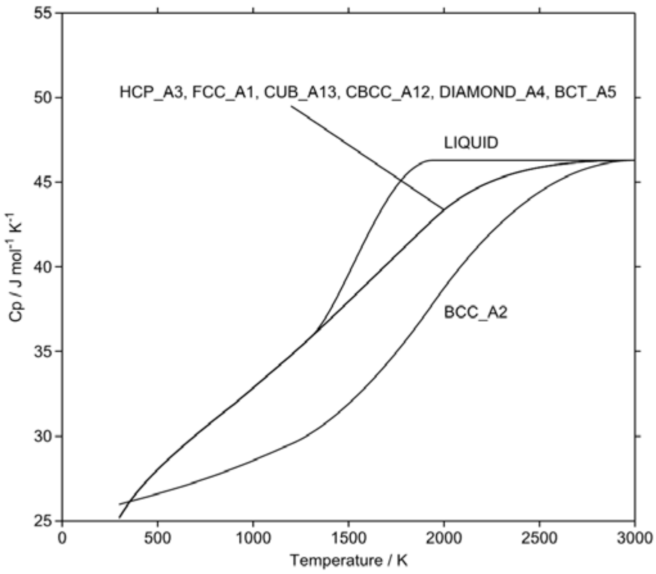
4602.2 *(298.15 < T < 4000)*

CUB_A13

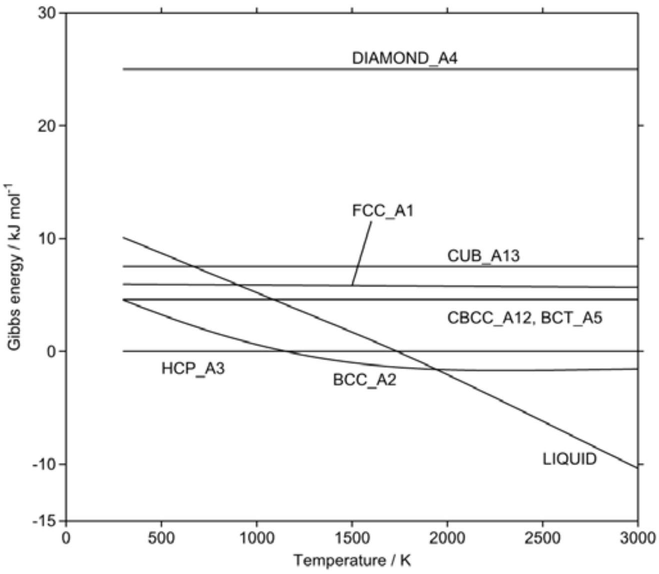
7531.2 *(298.15 < T < 4000)*

FCC_A1

6000 - 0.1 T *(298.15 < T < 4000)*



Heat capacity of Ti



Gibbs energy of phases of Ti relative to HCP_A3

Tl

Source of data: *I Ansara and N Saunders (unpublished work) [HCP_A3, BCC_A2]*
Hultgren [LIQUID]
Saunders et al. [FCC_A1]

HCP_A3

$-8104.038 + 107.140405\ T - 25.2274\ T\ \ln(T) - 3.3063E\text{-}3\ T^2 - 0.121807E\text{-}6\ T^3 + 42058\ T^{-1}$
(200 < T < 577)

$-15406.859 + 196.771926\ T - 38.4130658\ T\ \ln(T) + 5.228106E\text{-}3\ T^2 - 0.519136E\text{-}6\ T^3 + 729665\ T^{-1}$
(577 < T < 1800)

$-4885.034 + 106.361006\ T - 25.8437\ T\ ln(T) - 0.83662E\text{-}3\ T^2 + 0.000009E\text{-}6\ T^3 - 612570\ T^{-1}$
(1800 < T < 1801)

BCC_A2

$-9194.493 + 150.019517\ T - 33.0508\ T\ ln(T) + 17.2318E\text{-}3\ T^2 - 10.115933E\text{-}6\ T^3 + 82153\ T^{-1}$
(200 < T < 577)
$-41836.403 + 482.633817\ T - 79.2926704\ T\ ln(T) + 26.042993E\text{-}3\ T^2 - 2.359101E\text{-}6\ T^3 + 3507810\ T^{-1}$
(577 < T < 1800)
$-623.343 + 101.120182\ T - 25.8437\ T\ ln(T) - 0.83662E\text{-}3\ T^2 + 0.000009E\text{-}6\ T^3 - 612570\ T^{-1}$
(1800 < T < 1801)

LIQUID

$-946.623 + 0.755649\ T - 7.44455\ T\ ln(T) - 44.350292E\text{-}3\ T^2 + 14.248046E\text{-}6\ T^3 - 54228\ T^{-1}$
(200 < T < 577)
$-614.74 + 98.472609\ T - 25.8437\ T\ ln(T) - 0.83662E\text{-}3\ T^2 + 0.000009E\text{-}6\ T^3 - 612570\ T^{-1}$
(577 < T < 1801)

FCC_A1

$-7794.038 + 107.140405\ T - 25.2274\ T\ ln(T) - 3.3063E\text{-}3\ T^2 - 0.121807E\text{-}6\ T^3 + 42058\ T^{-1}$
(200 < T < 577)
$-15096.859 + 196.771926\ T - 38.4130658\ T\ ln(T) + 5.228106E\text{-}3\ T^2 - 0.519136E\text{-}6\ T^3 + 729665\ T^{-1}$
(577 < T < 1800)
$-4575.034 + 106.361006\ T - 25.8437\ T\ ln(T) - 0.83662E\text{-}3\ T^2 + 0.000009E\text{-}6\ T^3 - 612570\ T^{-1}$
(1800 < T < 1801)

Data relative to HCP_A3

BCC_A2

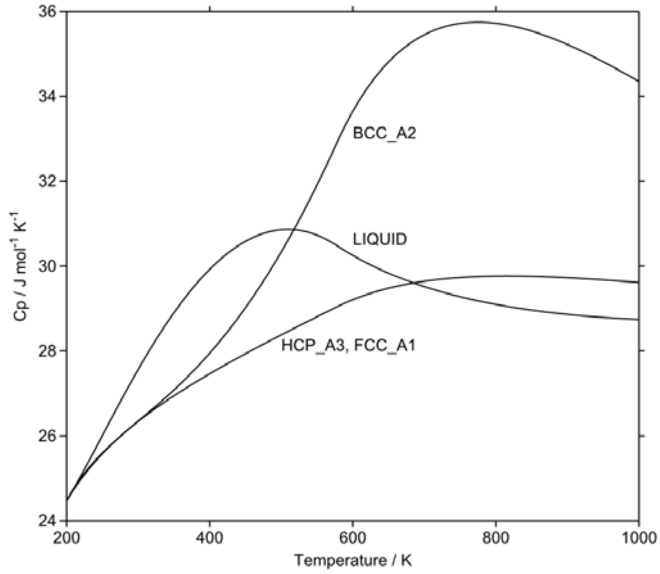
$-1090.455 + 42.879112\ T - 7.8234\ T\ ln(T) + 20.5381E\text{-}3\ T^2 - 9.994126E\text{-}6\ T^3 + 40095\ T^{-1}$
(200 < T < 577)
$-26429.544 + 285.861891\ T - 40.8796046\ T\ ln(T) + 20.814887E\text{-}3\ T^2 - 1.839965E\text{-}6\ T^3 + 2778145\ T^{-1}$
(577 < T < 1800)
$4261.691 - 5.240824\ T$ *(1800 < T < 1801)*

LIQUID

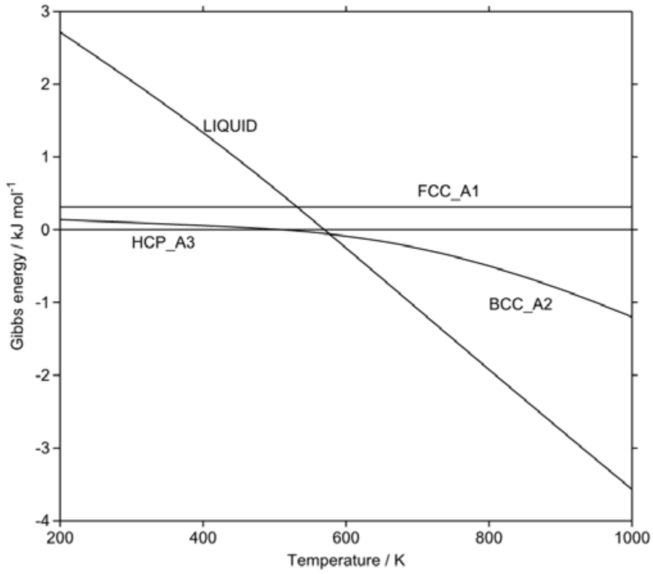
$7157.415 - 106.384756\ T + 17.78285\ T\ ln(T) - 41.043992E\text{-}3\ T^2 + 14.369853E\text{-}6\ T^3 - 96286\ T^{-1}$
(200 < T < 577)
$14792.119 - 98.299317\ T + 12.5693658\ T\ ln(T) - 6.064726E\text{-}3\ T^2 + 0.519145E\text{-}6\ T^3 - 1342235\ T^{-1}$
(577 < T < 1800)
$4270.294 - 7.888397\ T$ *(1800 < T < 1801)*

FCC_A1

310 *(200 < T < 1801)*



Heat capacity of Tl



Gibbs energy of phases of Tl relative to HCP_A3

Tm

Source of data: *Hultgren*

HCP_A3

$-10016.715 + 151.037648\ T - 34.3664974\ T\ln(T) + 12.110965E{-3}\ T^2 - 3.831156E{-6}\ T^3 + 95982\ T^{-1}$ *(298.15 < T < 700)*

$-14701.965 + 147.957496\ T - 32.1951269\ T\ln(T) + 0.444753E{-3}\ T^2 - 0.396694E{-6}\ T^3 + 1091664\ T^{-1}$ *(700 < T < 1600)*

$-8669.227 + 97.98144\ T - 25.1816969\ T\ln(T) - 3.384563E{-3}\ T^2$ *(1600 < T < 1818)*

$727125.608 - 4147.400632\ T + 534.082763\ T\ln(T) - 190.93039E{-3}\ T^2 + 11.689185E{-6}\ T^3 - 180382220\ T^{-1}$ *(1818 < T < 2300)*

LIQUID

$3182.534 + 144.479977\ T - 34.3664974\ T\ln(T) + 12.110965E{-3}\ T^2 - 3.831156E{-6}\ T^3 + 95982\ T^{-1}$ *(298.15 < T < 600)*

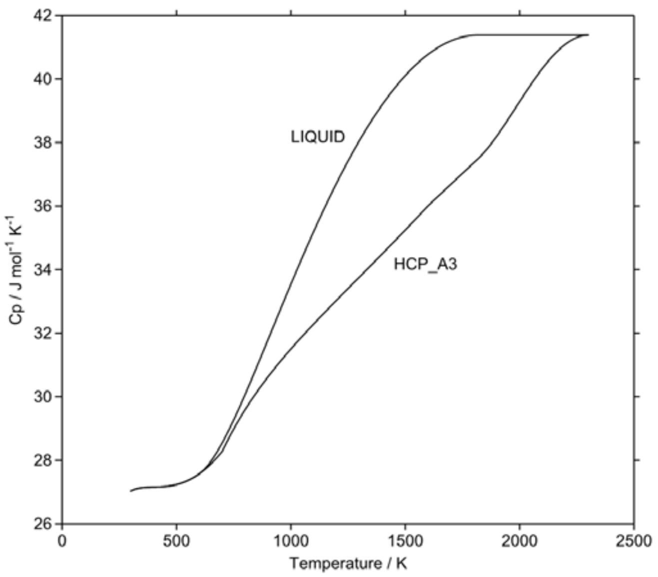
$22640.028 - 126.738485\ T + 6.8744933\ T\ln(T) - 25.487085E{-3}\ T^2 + 2.288172E{-6}\ T^3 - 1585412\ T^{-1}$ *(600 < T < 1818)*

$-10090.305 + 214.184413\ T - 41.37976\ T\ln(T)$ *(1818 < T < 2300)*

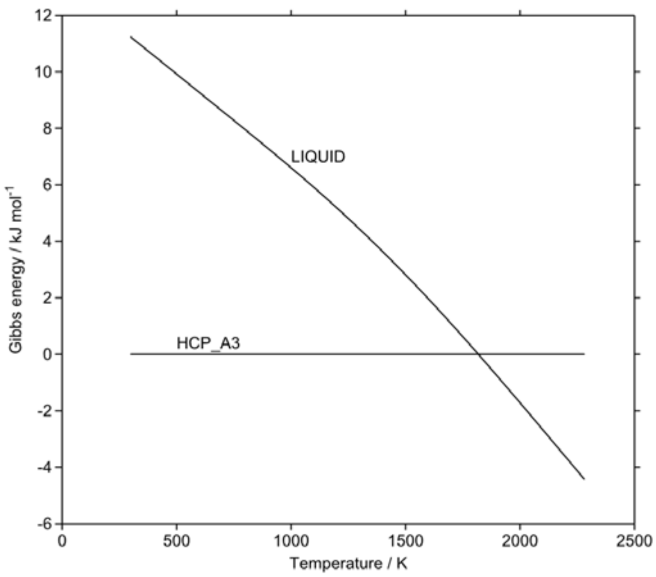
Data relative to HCP_A3

LIQUID

$13199.249 - 6.557671\ T$ *(298.15 < T < 600)*
$32656.743 - 277.776133\ T + 41.2409907\ T\ln(T) - 37.59805E\text{-}3\ T^2 + 6.119328E\text{-}6\ T^3 - 1681394\ T^{-1}$
(600 < T < 700)
$37341.993 - 274.695981\ T + 39.0696202\ T\ln(T) - 25.931838E\text{-}3\ T^2 + 2.684866E\text{-}6\ T^3 - 2677076\ T^{-1}$
(700 < T < 1600)
$31309.255 - 224.719925\ T + 32.0561902\ T\ln(T) - 22.102522E\text{-}3\ T^2 + 2.288172E\text{-}6\ T^3 - 1585412\ T^{-1}$
(1600 < T < 1818)
$-737215.913 + 4361.585045\ T - 575.462523\ T\ln(T) + 190.93039E\text{-}3\ T^2 - 11.689185E\text{-}6\ T^3$
$+ 180382220\ T^{-1}$ *(1818 < T < 2300)*



Heat capacity of Tm



Gibbs energy of phases of Tm relative to HCP_A3

U

Source of data: *M H Rand and A T Dinsdale (Unpublished work)*

ORTHORHOMBIC_A20

$-8407.734 + 130.955151\ T - 26.9182\ T\ln(T) + 1.25156E\text{-}3\ T^2 - 4.42605E\text{-}6\ T^3 + 38568\ T^{-1}$
(298.15 < T < 955)
$-22521.8 + 292.121093\ T - 48.66\ T\ln(T)$ *(955 < T < 3000)*

TETRAGONAL_U

$-5156.136 + 106.976316\ T - 22.841\ T\ln(T) - 10.84475E\text{-}3\ T^2 + 0.027889E\text{-}6\ T^3 + 81944\ T^{-1}$
(298.15 < T < 941.5)

$-14327.309 + 244.16802\ T - 42.9278\ T\ \ln(T)$ *(941.5 < T < 3000)*

BCC_A2

$-752.767 + 131.5381\ T - 27.5152\ T\ \ln(T) - 8.35595E{-3}\ T^2 + 0.967907E{-6}\ T^3 + 204611\ T^{-1}$
(298.15 < T < 1049)
$-4698.365 + 202.685635\ T - 38.2836\ T\ \ln(T)$ *(1049 < T < 3000)*

LIQUID

$3947.766 + 120.631251\ T - 26.9182\ T\ \ln(T) + 1.25156E{-3}\ T^2 - 4.42605E{-6}\ T^3 + 38568\ T^{-1}$
(298.15 < T < 955)
$-10166.3 + 281.797193\ T - 48.66\ T\ \ln(T)$ *(955 < T < 3000)*

FCC_A1

$-3407.734 + 130.955151\ T - 26.9182\ T\ \ln(T) + 1.25156E{-3}\ T^2 - 4.42605E{-6}\ T^3 + 38568\ T^{-1}$
(298.15 < T < 955)
$-17521.8 + 292.121093\ T - 48.66\ T\ \ln(T)$ *(955 < T < 3000)*

HCP_A3

$4247.233 + 131.5301\ T - 27.5152\ T\ \ln(T) - 8.35595E{-3}\ T^2 + 0.967907E{-6}\ T^3 + 204611\ T^{-1}$
(298.15 < T < 1049)
$301.635 + 202.677635\ T - 38.2836\ T\ \ln(T)$ *(1049 < T < 2500)*

Data relative to ORTHORHOMBIC_A20

TETRAGONAL_U

$3251.598 - 23.978835\ T + 4.0772\ T\ \ln(T) - 12.09631E{-3}\ T^2 + 4.453939E{-6}\ T^3 + 43376\ T^{-1}$
(298.15 < T < 941.5)
$-5919.575 + 113.212869\ T - 16.0096\ T\ \ln(T) - 1.25156E{-3}\ T^2 + 4.42605E{-6}\ T^3 - 38568\ T^{-1}$
(941.5 < T < 955)
$8194.491 - 47.953073\ T + 5.7322\ T\ \ln(T)$ *(955 < T < 3000)*

BCC_A2

$7654.967 + 0.582949\ T - 0.597\ T\ \ln(T) - 9.60751E{-3}\ T^2 + 5.393957E{-6}\ T^3 + 166043\ T^{-1}$
(298.15 < T < 955)
$21769.033 - 160.582993\ T + 21.1448\ T\ \ln(T) - 8.35595E{-3}\ T^2 + 0.967907E{-6}\ T^3 + 204611\ T^{-1}$
(955 < T < 1049)
$17823.435 - 89.435458\ T + 10.3764\ T\ \ln(T)$ *(1049 < T < 3000)*

LIQUID

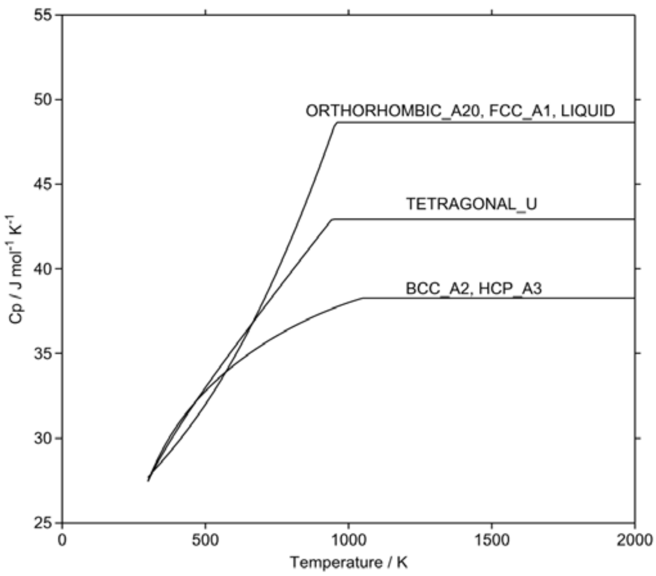
$12355.5 - 10.3239\ T$ *(298.15 < T < 3000)*

FCC_A1

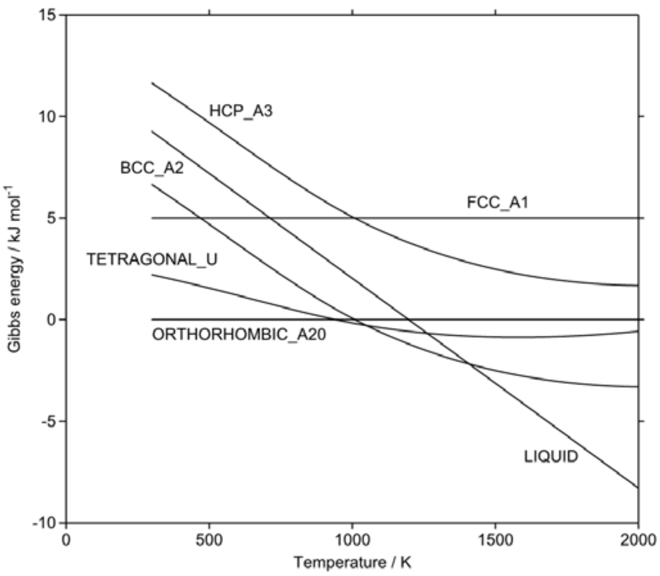
5000 *(298.15 < T < 3000)*

HCP_A3

12654.967 + 0.574949 T - 0.597 T ln(T) - 9.60751E-3 T^2 + 5.393957E-6 T^3 + 166043 T^{-1}
(298.15 < T < 955)
26769.033 - 160.590993 T + 21.1448 T ln(T) - 8.35595E-3 T^2 + 0.967907E-6 T^3 + 204611 T^{-1}
(955 < T < 1049)
22823.435 - 89.443458 T + 10.3764 T ln(T) *(1049 < T < 2500)*



Heat capacity of U



Gibbs energy of phases of U relative to ORTHORHOMBIC_A20

V

Source of data: *J Smith - Bull. Alloy Phase Diag. [BCC_A2, LIQUID]*
A Fernandez Guillermet, W Huang, Z. Metallkde., 1988, ***79****, 88. [FCC_A1, HCP_A3]*
Weiming Huang, TRITA-MAC-0439 [BCC_A12, CUB_A13]

BCC_A2

-7930.43 + 133.346053 T - 24.134 T ln(T) - 3.098E-3 T^2 + 0.12175E-6 T^3 + 69460 T^{-1}
(298.15 < T < 790)
-7967.842 + 143.291093 T - 25.9 T ln(T) + 0.0625E-3 T^2 - 0.68E-6 T^3 *(790 < T < 2183)*
-41689.864 + 321.140783 T - 47.43 T ln(T) + 644.389E29 T^{-9} *(2183 < T < 4000)*

LIQUID

$12833.687 + 123.890501\ T - 24.134\ T \ln(T) - 3.098E\text{-}3\ T^2 + 0.12175E\text{-}6\ T^3 + 69460\ T^{-1}$
$- 519.136E\text{-}24\ T^7$ *(298.15 < T < 790)*
$12796.275 + 133.835541\ T - 25.9\ T \ln(T) + 0.0625E\text{-}3\ T^2 - 0.68E\text{-}6\ T^3 - 519.136E\text{-}24\ T^7$
(790 < T < 2183)
$-19617.51 + 311.055983\ T - 47.43\ T \ln(T)$ *(2183 < T < 4000)*

CBCC_A12

$1069.57 + 133.346053\ T - 24.134\ T \ln(T) - 3.098E\text{-}3\ T^2 + 0.12175E\text{-}6\ T^3 + 69460\ T^{-1}$
(298.15 < T < 790)
$1032.158 + 143.291093\ T - 25.9\ T \ln(T) + 0.0625E\text{-}3\ T^2 - 0.68E\text{-}6\ T^3$ *(790 < T < 2183)*
$-32689.864 + 321.140783\ T - 47.43\ T \ln(T) + 644.389E29\ T^{-9}$ *(2183 < T < 4000)*

CUB_A13

$2069.57 + 133.346053\ T - 24.134\ T \ln(T) - 3.098E\text{-}3\ T^2 + 0.12175E\text{-}6\ T^3 + 69460\ T^{-1}$
(298.15 < T < 790)
$2032.158 + 143.291093\ T - 25.9\ T \ln(T) + 0.0625E\text{-}3\ T^2 - 0.68E\text{-}6\ T^3$ *(790 < T < 2183)*
$-31689.864 + 321.140783\ T - 47.43\ T \ln(T) + 644.389E29\ T^{-9}$ *(2183 < T < 4000)*

FCC_A1

$-430.43 + 135.046053\ T - 24.134\ T \ln(T) - 3.098E\text{-}3\ T^2 + 0.12175E\text{-}6\ T^3 + 69460\ T^{-1}$
(298.15 < T < 790)
$-467.842 + 144.991093\ T - 25.9\ T \ln(T) + 0.0625E\text{-}3\ T^2 - 0.68E\text{-}6\ T^3$ *(790 < T < 2183)*
$-34189.864 + 322.840783\ T - 47.43\ T \ln(T) + 644.389E29\ T^{-9}$ *(2183 < T < 4000)*

HCP_A3

$-3930.43 + 135.746053\ T - 24.134\ T \ln(T) - 3.098E\text{-}3\ T^2 + 0.12175E\text{-}6\ T^3 + 69460\ T^{-1}$
(298.15 < T < 790)
$-3967.842 + 145.691093\ T - 25.9\ T \ln(T) + 0.0625E\text{-}3\ T^2 - 0.68E\text{-}6\ T^3$ *(790 < T < 2183)*
$-37689.864 + 323.540783\ T - 47.43\ T \ln(T) + 644.389E29\ T^{-9}$ *(2183 < T < 4000)*

Data relative to BCC_A2

LIQUID

$20764.117 - 9.455552\ T - 519.136E\text{-}24\ T^7$ *(298.15 < T < 2183)*
$22072.354 - 10.0848\ T - 644.389E29\ T^{-9}$ *(2183 < T < 4000)*

CBCC_A12

9000 *(298.15 < T < 4000)*

CUB_A13

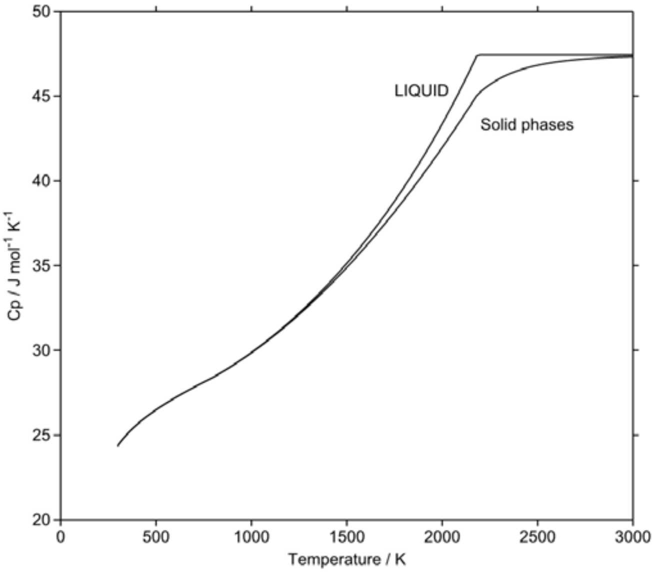
10000 *(298.15 < T < 4000)*

FCC_A1

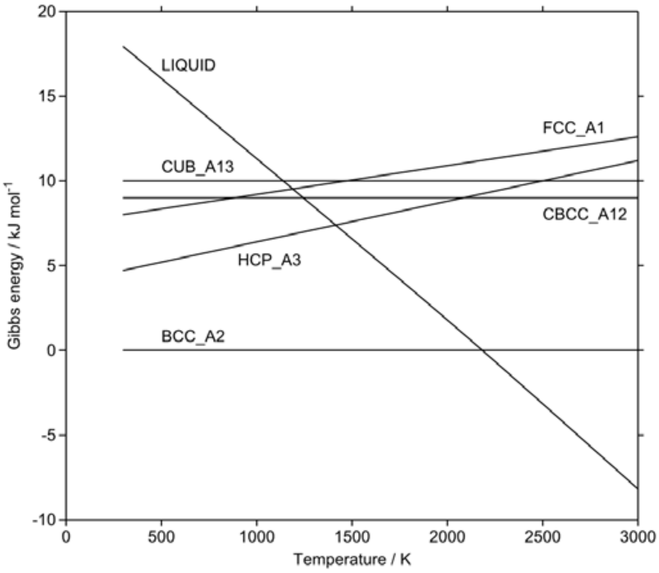
7500 + 1.7 T *(298.15 < T < 4000)*

HCP_A3

4000 + 2.4 T *(298.15 < T < 4000)*



Heat capacity of V



Gibbs energy of phases of V relative to BCC_A2

W

Source of data: *P Gustafson, Int. J. Thermophys., 1986,* ***6****, 395-409*

BCC_A2

$A = 9.5168E-6$ $a_0 = 9.386E-6$ $a_1 = 5.51E-9$
$K_0 = 3.1575E-12$ $K_1 = 1.6E-16$ $K_2 = 3.1E-20$ $n = 4$

$-7646.311 + 130.4\ T - 24.1\ T \ln(T) - 1.936E{-3}\ T^2 + 0.207E{-6}\ T^3 + 44500\ T^{-1} - 0.0533E{-9}\ T^4 + Gpres$ *(298.15 < T < 3695)*

$-82868.801 + 389.362335\ T - 54\ T \ln(T) + 1528.621E30\ T^{-9} + Gpres$ *(3695 < T < 6000)*

LIQUID

$A = 10.3E-6$ $a_0 = 9.386E-6$ $a_1 = 5.51E-9$
$K_0 = 3.1575E-12$ $K_1 = 1.6E-16$ $K_2 = 3.1E-20$ $n = 4$

$44514.273 + 116.29001\ T - 24.1\ T \ln(T) - 1.936E-3\ T^2 + 0.207E-6\ T^3 + 44500\ T^{-1} - 0.0533E-9\ T^4$
$- 2713.468E-27\ T^7 + Gpres$ *(298.15 < T < 3695)*
$-30436.051 + 375.175\ T - 54\ T \ln(T) + Gpres$ *(3695 < T < 6000)*

FCC_A1

$A = 9.5168E-6$ $a_0 = 9.386E-6$ $a_1 = 5.51E-9$
$K_0 = 3.1575E-12$ $K_1 = 1.6E-16$ $K_2 = 3.1E-20$ $n = 4$

$11653.689 + 131.03\ T - 24.1\ T \ln(T) - 1.936E-3\ T^2 + 0.207E-6\ T^3 + 44500\ T^{-1} - 0.0533E-9\ T^4 + Gpres$
(298.15 < T < 3695)
$-63568.801 + 389.992335\ T - 54\ T \ln(T) + 1528.621E30\ T^{-9} + Gpres$ *(3695 < T < 6000)*

HCP_A3

$A = 9.5168E-6$ $a_0 = 9.386E-6$ $a_1 = 5.51E-9$
$K_0 = 3.1575E-12$ $K_1 = 1.6E-16$ $K_2 = 3.1E-20$ $n = 4$

$7103.689 + 130.4\ T - 24.1\ T \ln(T) - 1.936E-3\ T^2 + 0.207E-6\ T^3 + 44500\ T^{-1} - 0.0533E-9\ T^4 + Gpres$
(298.15 < T < 3695)
$-68118.801 + 389.362335\ T - 54\ T \ln(T) + 1528.621E30\ T^{-9} + Gpres$ *(3695 < T < 6000)*

Data relative to BCC_A2

BCC_A2

$A = 9.5168E-6$ $a_0 = 9.386E-6$ $a_1 = 5.51E-9$
$K_0 = 3.1575E-12$ $K_1 = 1.6E-16$ $K_2 = 3.1E-20$ $n = 4$

Gpres *(298.15 < T < 6000)*

LIQUID

$A = 10.3E-6$ $a_0 = 9.386E-6$ $a_1 = 5.51E-9$
$K_0 = 3.1575E-12$ $K_1 = 1.6E-16$ $K_2 = 3.1E-20$ $n = 4$

$52160.584 - 14.10999\ T - 2713.468E-27\ T^7 + Gpres$ *(298.15 < T < 3695)*
$52432.75 - 14.187335\ T - 1528.621E30\ T^{-9} + Gpres$ *(3695 < T < 6000)*

FCC_A1

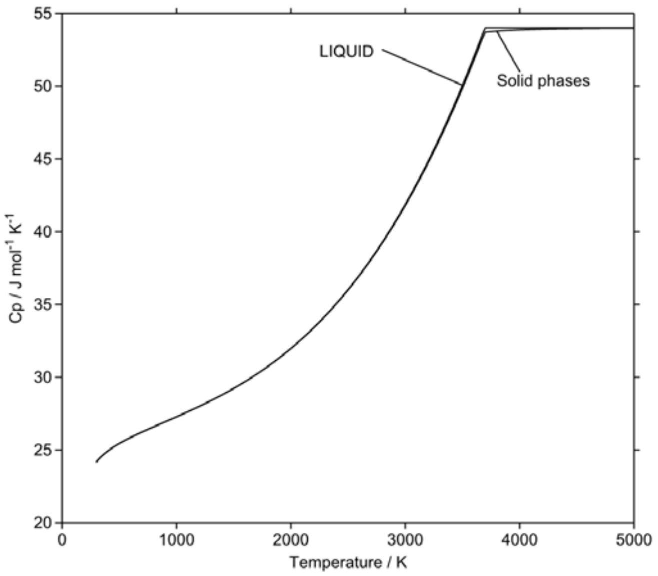
$A = 9.5168E-6$ $a_0 = 9.386E-6$ $a_1 = 5.51E-9$
$K_0 = 3.1575E-12$ $K_1 = 1.6E-16$ $K_2 = 3.1E-20$ $n = 4$

$19300 + 0.63\ T + Gpres$ *(298.15 < T < 6000)*

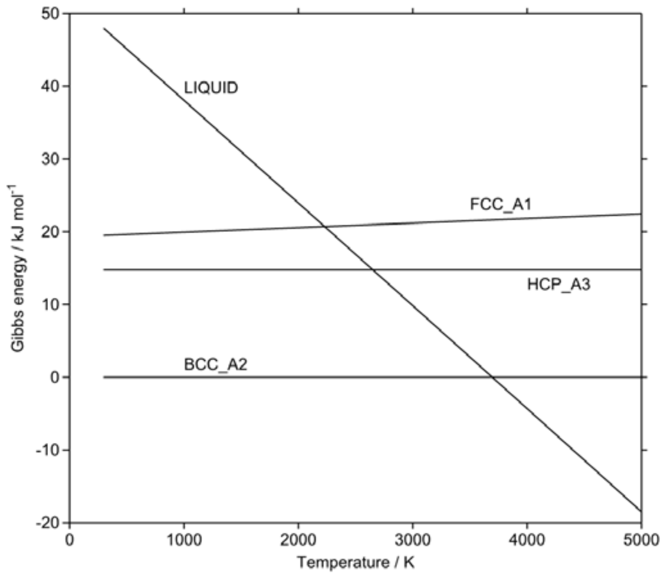
HCP_A3

A = 9.5168E-6 a_0 = 9.386E-6 a_1 = 5.51E-9
K_0 = 3.1575E-12 K_1 = 1.6E-16 K_2 = 3.1E-20 n = 4

14750 + Gpres *(298.15 < T < 6000)*



Heat capacity of W



Gibbs energy of phases of W relative to BCC_A2

Y

Source of data: *Huasen Shen, Weijing Zhang, Guoquan Liu, Run Wang and Zhenmin Du; Report F-95-03, May 1995, University of Science and Technology, Beijing [LIQUID, BCC_A2, HCP_A3]*
S G Fries, H L Lukas, unpublished work [FCC_A1]

HCP_A3

$-8011.094 + 128.572856\ T - 25.6656992\ T\ln(T) - 1.757164E\text{-}3\ T^2 - 0.417562E\text{-}6\ T^3 + 26912\ T^{-1}$
(100 < T < 1000)

$-7179.746 + 114.497104\ T - 23.4941827\ T\ln(T) - 3.82118E\text{-}3\ T^2 - 0.082535E\text{-}6\ T^3$
(1000 < T < 1795.15)

$-67480.776 + 382.124727\ T - 56.9527111\ T\ln(T) + 2.317744E\text{-}3\ T^2 - 0.072251E\text{-}6\ T^3 + 18077163\ T^{-1}$
(1795.15 < T < 3700)

BCC_A2

$-833.659 + 123.667346\ T - 25.5832578\ T\ln(T) - 2.37176E\text{-}3\ T^2 + 0.009104E\text{-}6\ T^3 + 27340\ T^{-1}$
(100 < T < 1000)

$-1297.798 + 134.528352\ T - 27.3038477\ T\ln(T) - 0.541758E\text{-}3\ T^2 - 0.305012E\text{-}6\ T^3$
(1000 < T < 1795.15)

$15389.497 + 0.981325\ T - 8.8829665\ T\ln(T) - 9.045766E{-3}\ T^2 + 0.402945E{-6}\ T^3 - 2542576\ T^{-1}$
(1795.15 < T < 3700)

LIQUID

$2098.507 + 119.41873\ T - 24.6467508\ T\ln(T) - 3.470235E{-3}\ T^2 - 0.812981E{-6}\ T^3 + 23714\ T^{-1}$
(100 < T < 1000)
$7386.448 + 19.452017\ T - 9.0681627\ T\ln(T) - 18.953337E{-3}\ T^2 + 1.759533E{-6}\ T^3$
(1000 < T < 1795.15)
$-12976.596 + 257.400783\ T - 43.0952\ T\ln(T)$ *(1795.15 < T < 3700)*

FCC_A1

$-2011.094 + 128.572856\ T - 25.6656992\ T\ln(T) - 1.757164E{-3}\ T^2 - 0.417562E{-6}\ T^3 + 26912\ T^{-1}$
(100 < T < 1000)
$-1179.746 + 114.497104\ T - 23.4941827\ T\ln(T) - 3.82118E{-3}\ T^2 - 0.082535E{-6}\ T^3$
(1000 < T < 1795.15)
$-61480.776 + 382.124727\ T - 56.9527111\ T\ln(T) + 2.317744E{-3}\ T^2 - 0.072251E{-6}\ T^3 + 18077163\ T^{-1}$
(1795.15 < T < 3700)

Data relative to HCP_A3

BCC_A2

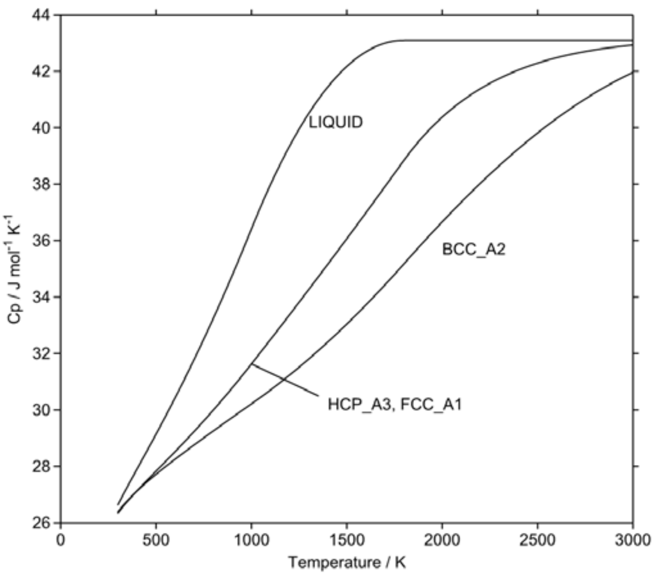
$7177.435 - 4.90551\ T + 0.0824414\ T\ln(T) - 0.614596E{-3}\ T^2 + 0.426666E{-6}\ T^3 + 429\ T^{-1}$
(100 < T < 1000)
$5881.947 + 20.031248\ T - 3.809665\ T\ln(T) + 3.279423E{-3}\ T^2 - 0.222478E{-6}\ T^3$ *(1000 < T < 1795.15)*
$82870.274 - 381.143402\ T + 48.0697446\ T\ln(T) - 11.36351E{-3}\ T^2 + 0.475196E{-6}\ T^3 - 20619739\ T^{-1}$
(1795.15 < T < 3700)

LIQUID

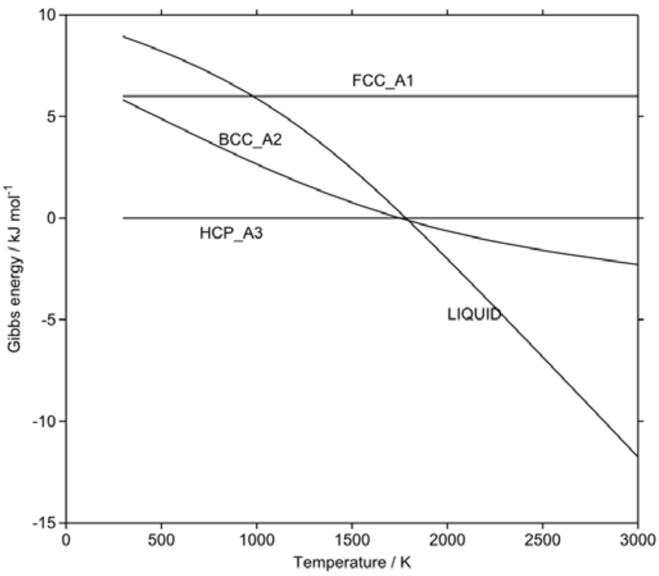
$10109.601 - 9.154126\ T + 1.0189484\ T\ln(T) - 1.71307E{-3}\ T^2 - 0.395419E{-6}\ T^3 - 3198\ T^{-1}$
(100 < T < 1000)
$14566.194 - 95.045087\ T + 14.42602\ T\ln(T) - 15.132157E{-3}\ T^2 + 1.842067E{-6}\ T^3$
(1000 < T < 1795.15)
$54504.18 - 124.723944\ T + 13.8575111\ T\ln(T) - 2.317744E{-3}\ T^2 + 0.072251E{-6}\ T^3 - 18077163\ T^{-1}$
(1795.15 < T < 3700)

FCC_A1

6000 *(100 < T < 3700)*



Heat capacity of Y



Gibbs energy of phases of Y relative to HCP_A3

Yb

Source of data: *Hultgren*

FCC_A1

$-9370.941 + 189.327664\ T - 40.0791\ T \ln(T) + 42.27115E\text{-}3\ T^2 - 22.242E\text{-}6\ T^3$ *(298.15 < T < 553)*
$-8192.154 + 121.065655\ T - 26.7591\ T \ln(T) - 2.56065E\text{-}3\ T^2$ *(553 < T < 1033)*
$16034.89 - 89.478241\ T + 2.7623966\ T \ln(T) - 17.961331E\text{-}3\ T^2 + 1.421719E\text{-}6\ T^3 - 3631462\ T^{-1}$
(1033 < T < 2000)

BCC_A2

$-965.99 - 21.293677\ T - 3.8534432\ T \ln(T) - 30.009694E\text{-}3\ T^2 + 4.743871E\text{-}6\ T^3 - 334650\ T^{-1}$
(298.15 < T < 1033)
$-13368.113 + 188.313864\ T - 36.1079\ T \ln(T)$ *(1033 < T < 1097)*
$-3911.847 + 113.174165\ T - 25.7402233\ T \ln(T) - 4.743348E\text{-}3\ T^2 + 0.363044E\text{-}6\ T^3 - 1553668\ T^{-1}$
(1097 < T < 2000)

LIQUID

$7030.788 - 40.615571\ T - 1.8061816\ T \ln(T) - 32.50938E\text{-}3\ T^2 + 5.136665E\text{-}6\ T^3 - 370554\ T^{-1}$
(298.15 < T < 1033)
$-6445.835 + 186.690398\ T - 36.7774\ T \ln(T)$ *(1033 < T < 2000)*

HCP_A3

$-4370.941 + 189.327664\ T - 40.0791\ T \ln(T) + 42.27115E\text{-}3\ T^2 - 22.242E\text{-}6\ T^3$ *(298.15 < T < 553)*
$-3192.154 + 121.065655\ T - 26.7591\ T \ln(T) - 2.56065E\text{-}3\ T^2$ *(553 < T < 1033)*

$21034.89 - 89.478241\ T + 2.7623966\ T\ln(T) - 17.961331E\text{-}3\ T^2 + 1.421719E\text{-}6\ T^3 - 3631462\ T^{-1}$
(1033 < T < 2000)

Data relative to FCC_A1

BCC_A2

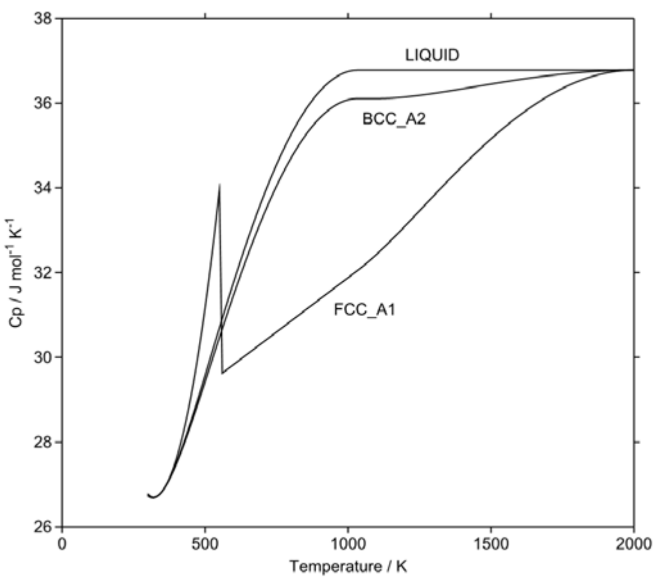
$8404.951 - 210.621341\ T + 36.2256568\ T\ln(T) - 72.280844E\text{-}3\ T^2 + 26.985871E\text{-}6\ T^3 - 334650\ T^{-1}$
(298.15 < T < 553)
$7226.164 - 142.359332\ T + 22.9056568\ T\ln(T) - 27.449044E\text{-}3\ T^2 + 4.743871E\text{-}6\ T^3 - 334650\ T^{-1}$
(553 < T < 1033)
$-29403.003 + 277.792105\ T - 38.8702966\ T\ln(T) + 17.961331E\text{-}3\ T^2 - 1.421719E\text{-}6\ T^3 + 3631462\ T^{-1}$
(1033 < T < 1097)
$-19946.737 + 202.652406\ T - 28.5026199\ T\ln(T) + 13.217983E\text{-}3\ T^2 - 1.058675E\text{-}6\ T^3 + 2077794\ T^{-1}$
(1097 < T < 2000)

LIQUID

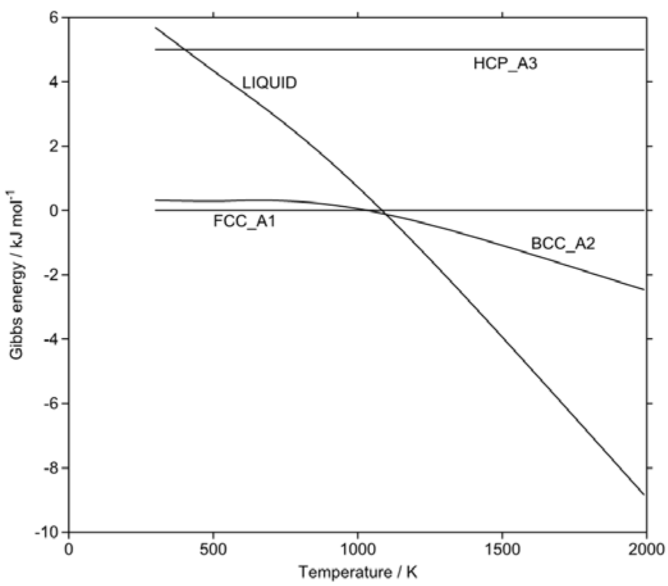
$16401.729 - 229.943235\ T + 38.2729184\ T\ln(T) - 74.78053E\text{-}3\ T^2 + 27.378665E\text{-}6\ T^3 - 370554\ T^{-1}$
(298.15 < T < 553)
$15222.942 - 161.681226\ T + 24.9529184\ T\ln(T) - 29.94873E\text{-}3\ T^2 + 5.136665E\text{-}6\ T^3 - 370554\ T^{-1}$
(553 < T < 1033)
$-22480.725 + 276.168639\ T - 39.5397966\ T\ln(T) + 17.961331E\text{-}3\ T^2 - 1.421719E\text{-}6\ T^3 + 3631462\ T^{-1}$
(1033 < T < 2000)

HCP_A3

5000 *(298.15 < T < 2000)*



Heat capacity of Yb



Gibbs energy of phases of Yb relative to FCC_A1

Zn

Source of data: *Hultgren [HCP_A3, LIQUID]*
S an Mey (Unpublished) [FCC_A1]
L Kaufman [BCC_A2]
COST507 database [BCT_A5, DIAMOND_A4]
A T Dinsdale, unpublished work [RHOMBOHEDRAL_A7]
B J Lee CALPHAD 1996, 20(4), 471-480 [TETRAGONAL_A6]
J Miettinen, CALPHAD 2004, 28(3), 313-320 [CUB_A13, CBCC_A12]
S.C. Hansen, CALPHAD 1998, 22, 359-373 [RHOMBO_A10]

HCP_ZN

$-7285.787 + 118.470069\,T - 23.701314\,T\ln(T) - 1.712034E\text{-}3\,T^2 - 1.264963E\text{-}6\,T^3$
(298.15 < T < 692.677)
$-11070.546 + 172.345644\,T - 31.38\,T\ln(T) + 470.47E24\,T^{-9}$ *(692.677 < T < 1700)*

LIQUID

$-128.565 + 108.177019\,T - 23.701314\,T\ln(T) - 1.712034E\text{-}3\,T^2 - 1.264963E\text{-}6\,T^3 - 358.949E\text{-}21\,T^7$
(298.15 < T < 692.677)
$-3620.385 + 161.60854\,T - 31.38\,T\ln(T)$ *(692.677 < T < 1700)*

HCP_A3

$-4315.967 + 116.900389\,T - 23.701314\,T\ln(T) - 1.712034E\text{-}3\,T^2 - 1.264963E\text{-}6\,T^3$
(298.15 < T < 692.677)
$-8100.726 + 170.775964\,T - 31.38\,T\ln(T) + 470.47E24\,T^{-9}$ *(692.677 < T < 1700)*

BCT_A5

$-4398.827 + 115.959669\,T - 23.701314\,T\ln(T) - 1.712034E\text{-}3\,T^2 - 1.264963E\text{-}6\,T^3$
(298.15 < T < 692.677)
$-8183.586 + 169.835244\,T - 31.38\,T\ln(T) + 470.47E24\,T^{-9}$ *(692.677 < T < 1700)*

DIAMOND_A4

$-7285.787 + 148.470069\,T - 23.701314\,T\ln(T) - 1.712034E\text{-}3\,T^2 - 1.264963E\text{-}6\,T^3$
(298.15 < T < 692.677)
$-11070.546 + 202.345644\,T - 31.38\,T\ln(T) + 470.47E24\,T^{-9}$ *(692.677 < T < 1700)*

RHOMBOHEDRAL_A7

$-4985.787 + 129.970069\,T - 23.701314\,T\ln(T) - 1.712034E\text{-}3\,T^2 - 1.264963E\text{-}6\,T^3$
(298.15 < T < 692.677)
$-8770.546 + 183.845644\,T - 31.38\,T\ln(T) + 470.47E24\,T^{-9}$ *(692.677 < T < 1700)*

TETRAGONAL_A6

$-3101.787 + 118.470069\ T - 23.701314\ T\ln(T) - 1.712034E\text{-}3\ T^2 - 1.264963E\text{-}6\ T^3$ *(298.15 < T < 692.677)*

$-6886.546 + 172.345644\ T - 31.38\ T\ln(T) + 470.47E24\ T^{-9}$ *(692.677 < T < 1700)*

BCC_A2

$-4398.827 + 115.959669\ T - 23.701314\ T\ln(T) - 1.712034E\text{-}3\ T^2 - 1.264963E\text{-}6\ T^3$ *(298.15 < T < 692.677)*

$-8183.586 + 169.835244\ T - 31.38\ T\ln(T) + 470.47E24\ T^{-9}$ *(692.677 < T < 1700)*

FCC_A1

$-4315.967 + 116.900389\ T - 23.701314\ T\ln(T) - 1.712034E\text{-}3\ T^2 - 1.264963E\text{-}6\ T^3$ *(298.15 < T < 692.677)*

$-8100.726 + 170.775964\ T - 31.38\ T\ln(T) + 470.47E24\ T^{-9}$ *(692.677 < T < 1700)*

CBCC_A12

$-5285.787 + 118.470069\ T - 23.701314\ T\ln(T) - 1.712034E\text{-}3\ T^2 - 1.264963E\text{-}6\ T^3$ *(298.15 < T < 692.677)*

$-9070.546 + 172.345644\ T - 31.38\ T\ln(T) + 470.47E24\ T^{-9}$ *(692.677 < T < 1700)*

CUB_A13

$-5285.787 + 118.470069\ T - 23.701314\ T\ln(T) - 1.712034E\text{-}3\ T^2 - 1.264963E\text{-}6\ T^3$ *(298.15 < T < 692.677)*

$-9070.546 + 172.345644\ T - 31.38\ T\ln(T) + 470.47E24\ T^{-9}$ *(692.677 < T < 1700)*

RHOMBO_A10

$-2128.565 + 118.177019\ T - 23.701314\ T\ln(T) - 1.712034E\text{-}3\ T^2 - 1.264963E\text{-}6\ T^3 - 358.949E\text{-}21\ T^7$ *(298.15 < T < 692.677)*

$-5620.385 + 171.60854\ T - 31.38\ T\ln(T)$ *(692.677 < T < 1700)*

Data relative to HCP_ZN

LIQUID

$7157.222 - 10.29305\ T - 358.949E\text{-}21\ T^7$ *(298.15 < T < 692.677)*

$7450.161 - 10.737104\ T - 470.47E24\ T^{-9}$ *(692.677 < T < 1700)*

HCP_A3

$2969.82 - 1.56968\ T$ *(298.15 < T < 1700)*

BCT_A5

2886.96 - 2.5104 T *(298.15 < T < 1700)*

DIAMOND_A4

30 T *(298.15 < T < 1700)*

RHOMBOHEDRAL_A7

2300 + 11.5 T *(298.15 < T < 1700)*

TETRAGONAL_A6

4184 *(298.15 < T 1700)*

BCC_A2

2886.96 - 2.5104 T *(298.15 < T 1700)*

FCC_A1

2969.82 - 1.56968 T *(298.15 < T < 1700)*

CBCC_A12

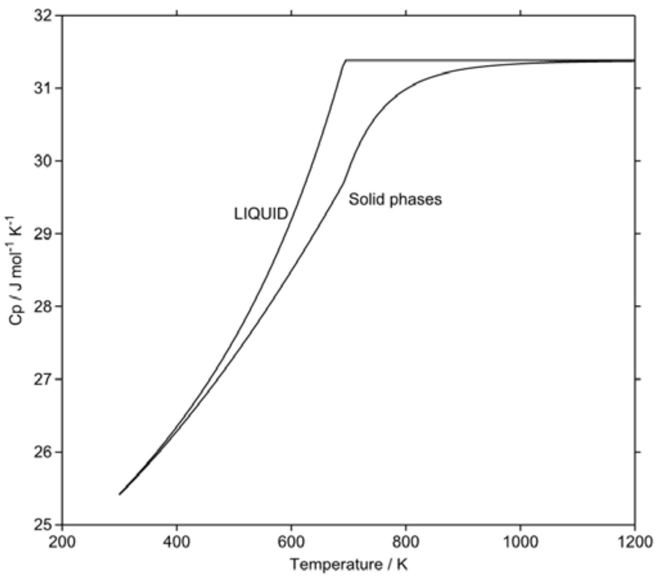
2000 *(298.15 < T < 1700)*

CUB_A13

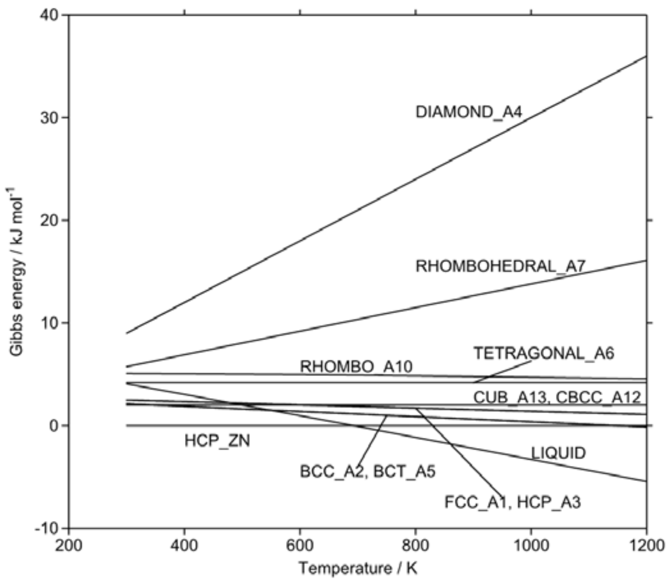
2000 *(298.15 < T < 1700)*

RHOMBO_A10

5157.222 - 0.29305 T - 358.949E-21 T^7 *(298.15 < T < 692.677)*
5450.161 - 0.737104 T - 470.47E24 T^{-9} *(692.677 < T < 1700)*



Heat capacity of Zn



Gibbs energy of phases of Zn relative to HCP_ZN

Zr

Source of data: *A Fernandez Guillermet, High Temp. - High Press., 1987, **19**, 119-60 [HCP_A3, BCC_A2, OMEGA, LIQUID]*
Saunders et al. [FCC_A1]

HCP_A3

A = 13.9567E-6 a_0 = 12.443E-6 a_1 = 14.76E-9
K_0 = 1.0063E-11 K_1 = 1.573E-15 n = 3.006

-7827.595 + 125.64905 T - 24.1618 T ln(T) - 4.37791E-3 T^2 + 34971 T^{-1} + Gpres *(130 < T < 2128)*
-26085.921 + 262.724183 T - 42.144 T ln(T) - 1342.896E28 T^{-9} + Gpres *(2128 < T < 6000)*

BCC_A2

A = 13.7141E-6 a_0 = 3.0381E-5
K_0 = 1.0063E-11 K_1 = 1.573E-15 n = 3.006

-525.539 + 124.9457 T - 25.607406 T ln(T) - 0.340084E-3 T^2 - 0.009729E-6 T^3 + 25233 T^{-1}
- 0.076143E-9 T^4 + Gpres *(298.15 < T < 2128)*
-30705.955 + 264.284163 T - 42.144 T ln(T) + 1276.058E29 T^{-9} + Gpres *(2128 < T < 6000)*

LIQUID

A = 1.44092E-5 a_0 = 3.0381E-5
K_0 = 1.0063E-11 K_1 = 1.573E-15 n = 3.006

10320.095 + 116.568238 T - 24.1618 T ln(T) - 4.37791E-3 T^2 + 34971 T^{-1}+ 1627.5E-25 T^7 + Gpres
(298.15 < T < 2128)

$-8281.26 + 253.812609\ T - 42.144\ T\ln(T) + Gpres$ *(2128 < T < 6000)*

OMEGA

$A = 1.37115E\text{-}5$ $a_0 = 3.0381E\text{-}5$
$K_0 = 1.0063E\text{-}11$ $K_1 = 1.573E\text{-}15$ $n = 3.006$

$-8878.082 + 144.432234\ T - 26.8556\ T\ln(T) - 2.799446E\text{-}3\ T^2 + 38376\ T^{-1} + Gpres$ *(298.15 < T < 2128)*
$-29500.524 + 265.290858\ T - 42.144\ T\ln(T) + 717.445E29\ T^{-9} + Gpres$ *(2128 < T < 6000)*

ORTHORHOMBIC_A20

$4474.461 + 124.9457\ T - 25.607406\ T\ln(T) - 0.340084E\text{-}3\ T^2 - 0.009729E\text{-}6\ T^3 + 25233\ T^{-1} - 0.076143E\text{-}9\ T^4$ *(298.15 < T < 2128)*
$-25705.955 + 264.284163\ T - 42.144\ T\ln(T) + 1276.058E29\ T^{-9}$ *(2128 < T < 2500)*

TETRAGONAL_U

$4474.461 + 124.9457\ T - 25.607406\ T\ln(T) - 0.340084E\text{-}3\ T^2 - 0.009729E\text{-}6\ T^3 + 25233\ T^{-1} - 0.076143E\text{-}9\ T^4$ *(298.15 < T < 2128)*
$-25705.955 + 264.284163\ T - 42.144\ T\ln(T) + 1276.058E29\ T^{-9}$ *(2128 < T < 2500)*

CBCC_A12

$-3225.395 + 125.64905\ T - 24.1618\ T\ln(T) - 4.37791E\text{-}3\ T^2 + 34971\ T^{-1}$ *(298.15 < T < 2128)*
$-21483.721 + 262.724183\ T - 42.144\ T\ln(T) - 1342.896E28\ T^{-9}$ *(2128 < T < 6000)*

CUB_A13

$-296.395 + 125.64905\ T - 24.1618\ T\ln(T) - 4.37791E\text{-}3\ T^2 + 34971\ T^{-1}$ *(298.15 < T < 2128)*
$-18554.721 + 262.724183\ T - 42.144\ T\ln(T) - 1342.896E28\ T^{-9}$ *(2128 < T < 6000)*

FCC_A1

$-227.595 + 124.74905\ T - 24.1618\ T\ln(T) - 4.37791E\text{-}3\ T^2 + 34971\ T^{-1}$ *(298.15 < T < 2128)*
$-18485.921 + 261.824183\ T - 42.144\ T\ln(T) - 1342.896E28\ T^{-9}$ *(2128 < T < 6000)*

Data relative to HCP_A3

HCP_A3

$A = 13.9567E\text{-}6$ $a_0 = 12.443E\text{-}6$ $a_1 = 14.76E\text{-}9$
$K_0 = 1.0063E\text{-}11$ $K_1 = 1.573E\text{-}15$ $n = 3.006$

Gpres *(130.00 < T < 6000)*

BCC_A2

$A = 13.7141E\text{-}6$ $a_0 = 3.0381E\text{-}5$
$K_0 = 1.0063E\text{-}11$ $K_1 = 1.573E\text{-}15$ $n = 3.006$

$7302.056 - 0.70335\ T - 1.445606\ T \ln(T) + 4.037826E\text{-}3\ T^2 - 0.009729E\text{-}6\ T^3 - 9738\ T^{-1}$
$- 0.076143E\text{-}9\ T^4 + Gpres$ *(298.15 < T < 2128)*
$-4620.034 + 1.55998\ T + 1410.348E29\ T^{-9} + Gpres$ *(2128 < T < 6000)*

LIQUID

$A = 1.44092E\text{-}5$ $a_0 = 3.0381E\text{-}5$
$K_0 = 1.0063E\text{-}11$ $K_1 = 1.573E\text{-}15$ $n = 3.006$

$18147.69 - 9.080812\ T + 1627.5E\text{-}25\ T^7 + Gpres$ *(298.15 < T < 2128)*
$17804.661 - 8.911574\ T + 1342.896E28\ T^{-9} + Gpres$ *(2128 < T < 6000)*

OMEGA

$A = 1.37115E\text{-}5$ $a_0 = 3.0381E\text{-}5$
$K_0 = 1.0063E\text{-}11$ $K_1 = 1.573E\text{-}15$ $n = 3.006$

$-1050.487 + 18.783184\ T - 2.6938\ T \ln(T) + 1.578464E\text{-}3\ T^2 + 3405\ T^{-1} + Gpres$ *(298.15 < T < 2128)*
$-3414.603 + 2.566675\ T + 851.735E29\ T^{-9} + Gpres$ *(2128 < T < 6000)*

ORTHORHOMBIC_A20

$12302.056 - 0.70335\ T - 1.445606\ T \ln(T) + 4.037826E\text{-}3\ T^2 - 0.009729E\text{-}6\ T^3 - 9738\ T^{-1}$
$- 0.076143E\text{-}9\ T^4$ *(298.15 < T < 2128)*
$379.966 + 1.55998\ T + 1410.348E29\ T^{-9}$ *(2128 < T < 2500)*

TETRAGONAL_U

$12302.056 - 0.70335\ T - 1.445606\ T \ln(T) + 4.037826E\text{-}3\ T^2 - 0.009729E\text{-}6\ T^3 - 9738\ T^{-1}$
$- 0.076143E\text{-}9\ T^4$ *(298.15 < T < 2128)*
$379.966 + 1.55998\ T + 1410.348E29\ T^{-9}$ *(2128 < T < 2500)*

CBCC_A12

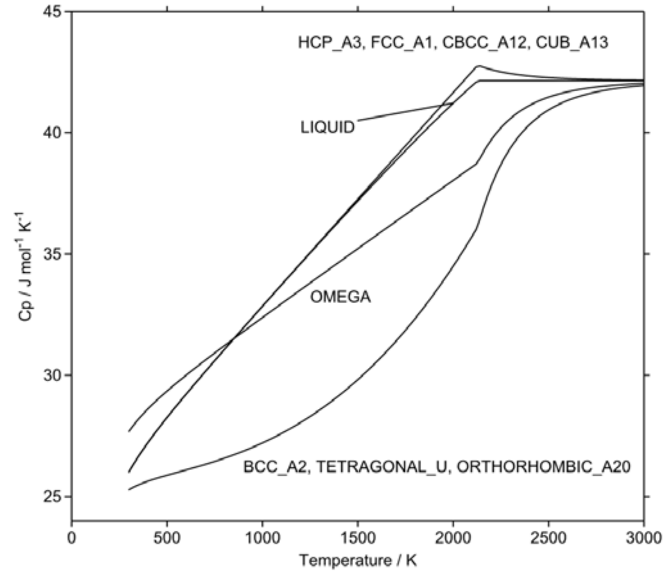
4602.2 *(298.15 < T < 6000)*

CUB_A13

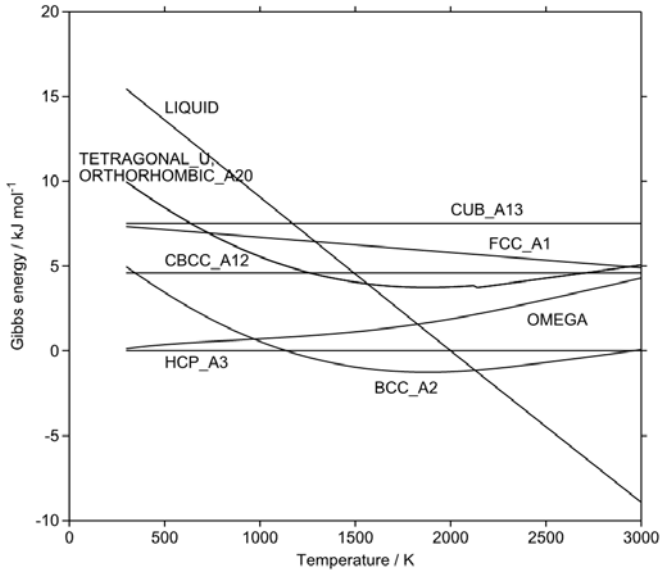
7531.2 *(298.15 < T < 6000)*

FCC_A1

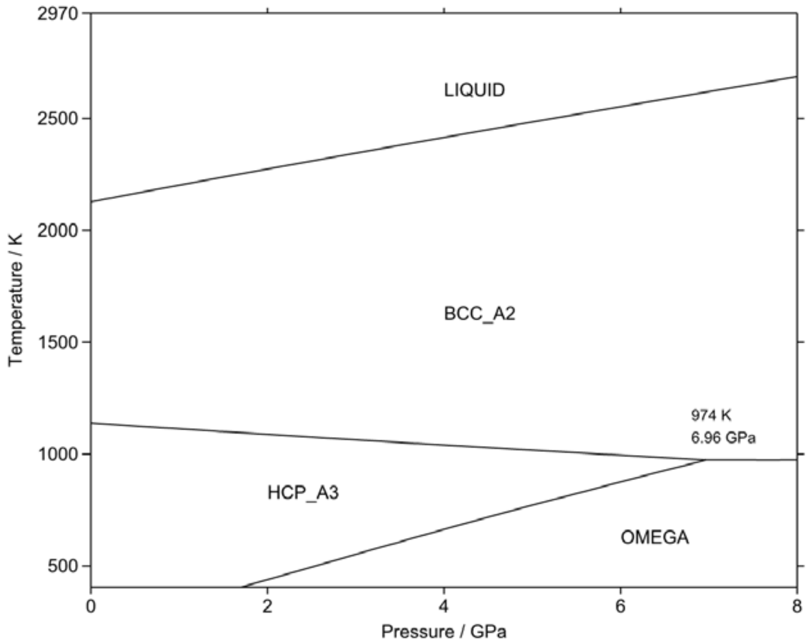
7600 - 0.9 T *(298.15 < T < 6000)*



Heat capacity of Zr



Gibbs energy of phases of Zr relative to HCP_A3



P-T phase diagram for Zr