calcium

Inchi: InChI=1S/Ca
InchiKey: OYPRJOBELJOOCE-UHFFFAOYSA-N
Formula: Ca
SMILES: [Ca]
Mol. weight [g/mol]: 40.08
CAS: 7440-70-2

Physical Properties

Property code	Value	Unit	Source
ea	0.02 ± 0.00	eV	NIST Webbook
ea	0.02 ± 0.00	eV	NIST Webbook
ea	0.02 ± 0.00	eV	NIST Webbook
ea	0.04 ± 0.01	eV	NIST Webbook
hf	177.80 ± 0.80	kJ/mol	NIST Webbook
ie	6.00 ± 0.30	eV	NIST Webbook
ie	6.11	eV	NIST Webbook
ie	6.00 ± 0.30	eV	NIST Webbook
ie	6.11	eV	NIST Webbook
ie	6.11 ± 0.00	eV	NIST Webbook
ie	6.08 ± 0.06	eV	NIST Webbook
ie	6.11 ± 0.00	eV	NIST Webbook
ie	6.06 ± 0.05	eV	NIST Webbook
ie	6.11 ± 0.00	eV	NIST Webbook
ie	6.10	eV	NIST Webbook
ie	6.11	eV	NIST Webbook
ie	6.11	eV	NIST Webbook
ie	6.21 ± 0.09	eV	NIST Webbook
sgb	154.89 ± 0.00	J/mol×K	NIST Webbook
ss	41.59 ± 0.40	J/mol×K	NIST Webbook
tb	1757.00 ± 2.00	K	NIST Webbook
tt	1112.90 ± 2.00	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43468e+01
Coeff. B	-1.60244e+04
Coeff. C	-1.10230e+02
Temperature range (K), min.	864.15
Temperature range (K), max.	1755.15

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Standard molar enthalpies of formation of hydroxy-, chlor-, and bromapatite:	https://www.doi.org/10.1016/j.jct.2005.01.010
Calorimetric studies and thermodynamic properties of liquid Ag-Ca alloys:	https://www.doi.org/10.1016/j.jct.2014.05.021
Standard enthalpy, entropy and Gibbs free energy of formation of "A" type carbonate phosphocalcium hydroxyapatites:	https://www.doi.org/10.1016/j.jct.2016.10.035
Thermochemical properties of two mixed alkali-alkaline earth metal borates with NLO properties for Ba2LiB5O10 and LiCaB3O6:	https://www.doi.org/10.1016/j.jct.2018.02.020
Thermodynamic stability of Ca3TeO6 determined by a solid electrolyte EMF method:	https://www.doi.org/10.1016/j.tca.2015.07.001
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7440702&Units=SI

Legend

ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
pvap:	Vapor pressure
sgb:	Molar entropy at standard conditions (1 bar)
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tt:	Triple Point Temperature