Titanium tetrachloride

Other names:	Tetrachlorure de titane
	TiCl4
	Titaantetrachloride
	Titanic chloride
	Titanium chloride
	Titanium chloride (TiCl4)
	Titanium chloride (TiCl4) (T-4)-
	Titanium(IV) chloride
	Titanium(IV)tetrachloride
	Titantetrachlorid
	UN 1838
Inchi:	InChI=1S/4ClH.Ti/h4*1H;/q;;;;+4/p-4
InchiKey:	XJDNKRIXUMDJCW-UHFFFAOYSA-J
Formula:	Cl4Ti
SMILES:	Cl[Ti](Cl)(Cl)Cl
Mol. weight [g/mol]:	189.68
CAS:	7550-45-0

Physical Properties

Property code	Value	Unit	Source
ea	2.88 ± 0.15	eV	NIST Webbook
hf	-763.20 ± 3.00	kJ/mol	NIST Webbook
ie	11.70	eV	NIST Webbook
ie	11.50	eV	NIST Webbook
ie	11.65 ± 0.15	eV	NIST Webbook
ie	11.69	eV	NIST Webbook
ie	11.76	eV	NIST Webbook
ie	11.78 ± 0.04	eV	NIST Webbook
ie	11.70	eV	NIST Webbook
rhoc	570.93 ± 7.59	kg/m3	NIST Webbook
sgb	353.20 ± 4.00	J/mol×K	NIST Webbook
tb	407.95 ± 1.00	K	NIST Webbook
tc	639.10 ± 0.60	K	NIST Webbook
tf	248.64 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	37.50	kJ/mol	336.50	NIST Webbook
hvapt	37.90	kJ/mol	389.00	NIST Webbook
hvapt	39.80	kJ/mol	335.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47824e+01
Coeff. B	-3.84261e+03
Coeff. C	-3.09400e+01
Temperature range (K), min.	249.05
Temperature range (K), max.	638.00

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7550450&Units=SI

Legend

ea: Electron affinity
hf: Enthalpy of formation at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
pvap: Vapor pressure
rhoc: Critical density
sgb: Molar entropy at standard conditions (1 bar)
tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point