Titanocene dichloride

Other names:	Bis(cyclopentadienyl)dichlorotitanium
	Bis(cyclopentadienyl)titanium dichloride
	Bis(«pi»-cyclopentadienyl)dichlorotitanium
	Bis(«pi»-cyclopentadienyl)titanium dichloride
	Bis(Â«piÂ»-cyclopentadienyl)dichlorotitanium
	Bis(Â«piÂ»-cyclopentadienyl)titanium dichloride
	Dichlorobis(1,3-cyclopentadiene)titanium
	Dichlorobis(cyclopentadienyl)titanium
	Dichlorobis(«eta»5-2,4-cyclopentadien-1-yl)titanium
	Dichlorobis(«eta»5-cyclopentadienyl)titanium
	Dichlorobis(«pi»-cyclopentadienyl)titanium
	Dichlorobis(Â«etaÂ»5-2,4-cyclopentadien-1-yl)titanium
	Dichlorobis(Â«etaÂ»5-cyclopentadienyl)titanium
	Dichlorobis(Â«piÂ»-cyclopentadienyl)titanium
	Dichlorodi-«pi»-cyclopentadienyltitanium
	Dichlorodi-Â«piÂ»-cyclopentadienyltitanium
	Dichlorodicyclopentadienyltitanium
	Dichlorotitanocene
	Dicyclopentadienyldichlorotitanium
	Dicyclopentadienyltitanium dichloride
	NCI-C04502
	NSC 78453
	Titanium, bis(cyclopentadienyl)dichloride-
	Titanium, dichlorobis(«eta»5-2,4-cyclopentadien-1-yl)-
	Titanium, dichlorobis(Â«etaÂ»5-2,4-cyclopentadien-1-yl)-
	Titanium, dichlorodi-«pi»-cyclopentadienyl-
	Titanium, dichlorodi-Â«piÂ»-cyclopentadienyl-
	bis(«eta»5-Cyclopentadienyl)titanium dichloride
	bis(Â«etaÂ»5-Cyclopentadienyl)titanium dichloride
	dichlorobis(«eta»-cyclopentadienyl)titanium
	dichlorobis(Â«etaÂ»-cyclopentadienyl)titanium
Inchi:	InChI=1S/2C5H5.2ClH.Ti/c2*1-2-4-5-3-1;;;/h2*1-5H;2*1H;/q;;;;+2/p-2
InchiKey:	XKLWATAZDMHTSH-UHFFFAOYSA-L
Formula:	C10H10Cl2Ti
SMILES:	Cl[Ti]12345678(Cl)(C9C1C2C3C94)C1C5C6C7C18
Mol. weight [g/mol]:	248.96
CAS:	1271-19-8

Physical Properties

Property code	Value	Unit	Source
chs	-5971.40 ± 7.50	kJ/mol	NIST Webbook
chs	-5849.00 ± 21.00	kJ/mol	NIST Webbook
chs	-5715.00 ± 21.00	kJ/mol	NIST Webbook
hf	-542.00 ± 21.00	kJ/mol	NIST Webbook
hf	-564.00 ± 21.00	kJ/mol	NIST Webbook
hf	-264.80 ± 8.00	kJ/mol	NIST Webbook
hfs	-661.00 ± 21.00	kJ/mol	NIST Webbook
hfs	-639.00 ± 21.00	kJ/mol	NIST Webbook
hfs	-383.60 ± 7.70	kJ/mol	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.50 ± 0.10	eV	NIST Webbook
ie	8.46 ± 0.05	eV	NIST Webbook
ie	8.98 ± 0.16	eV	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	124.40	kJ/mol	475.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.84254e+01
Coeff. B	-1.49668e+04
Temperature range (K), min.	531.91
Temperature range (K), max.	647.52

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1271198&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
ie:	Ionization energy
pvap:	Vapor pressure