Phenyl trichlorosilane

Other names:	CP0280
	Phenylsilicon trichloride
	Silane, phenyltrichloro-
	Silane, trichlorophenyl-
	Silicon phenyl trichloride
	Trichlorophenylsilane
	UN 1804
Inchi:	InChI=1S/C6H5Cl3Si/c7-10(8,9)6-4-2-1-3-5-6/h1-5H
InchiKey:	ORVMIVQULIKXCP-UHFFFAOYSA-N
Formula:	C6H5Cl3Si
SMILES:	Cl[Si](Cl)(Cl)c1ccccc1
Mol. weight [g/mol]:	211.55
CAS:	98-13-5

Physical Properties

Property code	Value	Unit	Source
ie	9.10	eV	NIST Webbook
ie	9.55	eV	NIST Webbook
log10ws	-5.09		Crippen Method
logp	2.549		Crippen Method
rinpol	1144.00		NIST Webbook
rinpol	1144.00		NIST Webbook
sl	314.70	J/mol×K	NIST Webbook
tb	474.00	K	NIST Webbook
tt	233.40 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	220.70	J/mol×K	298.15	NIST Webbook
hfust	11.66	kJ/mol	233.40	NIST Webbook
hfust	11.66	kJ/mol	233.40	NIST Webbook
hfust	11.66	kJ/mol	233.40	NIST Webbook
hvapt	51.10	kJ/mol	393.00	NIST Webbook

hvapt	47.90	kJ/mol	422.50	NIST Webbook
sfust	49.96	J/mol×K	233.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45369e+01
Coeff. B	-4.07367e+03
Coeff. C	-6.42400e+01
Temperature range (K), min.	350.12
Temperature range (K), max.	505.81

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C98135&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpl: Liquid phase heat capacity
hfust: Enthalpy of fusion at a given temperature
hvapt: Enthalpy of vaporization at a given temperature
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
pvap: Vapor pressure
rinpol: Non-polar retention indices
sfust: Entropy of fusion at a given temperature
sl: Liquid phase molar entropy at standard conditions
tb: Normal Boiling Point Temperature
tt: Triple Point Temperature