Methanesulfenyl chloride, trichloro-

Other names:	(Trichloromethane)sulfenyl chloride
	(Trichloromethyl)sulfenyl chloride
	Perchloromethyl mercaptan
	Clairsit
	Mercaptan methylique perchlore
	Perchlormethylmerkaptan
	PCM
	Rcra waste number P118
	Trichloromethanesulphenyl chloride
	Trichloromethylsulphenyl chloride
	UN 1670
	NSC 66404
	Perchloromethanethiol
Inchi:	InChI=1S/CCl4S/c2-1(3,4)6-5
InchiKey:	RYFZYYUIAZYQLC-UHFFFAOYSA-N
Formula:	CCl4S
SMILES:	ClSC(Cl)(Cl)Cl
Mol. weight [g/mol]:	185.89
CAS:	594-42-3

Physical Properties

Property code	Value	Unit	Source
gf	-54.22	kJ/mol	Joback Method
hf	-93.81	kJ/mol	Joback Method
hfl	-75.70	kJ/mol	NIST Webbook
hfus	11.85	kJ/mol	Joback Method
hvap	40.88	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.201		Crippen Method
mcvol	90.260	ml/mol	McGowan Method
pc	4917.69	kPa	Joback Method
tb	437.55	K	Joback Method
tc	684.95	K	Joback Method
tf	257.53	K	Joback Method
vc	0.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	116.50	J/mol×K	437.55	Joback Method
cpg	119.54	J/mol×K	478.78	Joback Method
cpg	122.16	J/mol×K	520.02	Joback Method
cpg	124.37	J/mol×K	561.25	Joback Method
cpg	126.21	J/mol×K	602.48	Joback Method
cpg	127.73	J/mol×K	643.72	Joback Method
cpg	128.95	J/mol×K	684.95	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C594423&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume