Methanesulfenylchloride

Inchi: InChI=1S/CH3ClS/c1-3-2/h1H3
InchiKey: DDCYYCUMAFYDDU-UHFFFAOYSA-N
Formula: CH3ClS
SMILES: CSCl
Mol. weight [g/mol]: 82.55
CAS: 5813-48-9

Physical Properties

Property code	Value	Unit	Source
gf	-21.27	kJ/mol	Joback Method
hf	-37.84	kJ/mol	Joback Method
hfus	6.67	kJ/mol	Joback Method
hvap	29.02	kJ/mol	Joback Method
ie	9.20 ± 0.10	eV	NIST Webbook
log10ws	-1.27		Crippen Method
logp	1.503		Crippen Method
mcvol	53.540	ml/mol	McGowan Method
pc	5619.38	kPa	Joback Method
tb	328.49	K	Joback Method
tc	531.63	K	Joback Method
tf	165.35	K	Joback Method
vc	0.195	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	65.52	J/mol×K	328.49	Joback Method
cpg	68.44	J/mol×K	362.35	Joback Method
cpg	71.29	J/mol×K	396.20	Joback Method
cpg	74.06	J/mol×K	430.06	Joback Method
cpg	76.75	J/mol×K	463.92	Joback Method
cpg	79.37	J/mol×K	497.77	Joback Method
cpg	81.90	J/mol×K	531.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5813489&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
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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