Chlorothioformylsulfenylchloride

Inchi: InChI=1S/CCl2S2/c2-1(4)5-3
InchiKey: COAQRZPGAKEOHU-UHFFFAOYSA-N
Formula: CCl2S2
SMILES: S=C(Cl)SCl
Mol. weight [g/mol]: 147.05
CAS: 72087-91-3

Physical Properties

Property code	Value	Unit	Source
gf	83.86	kJ/mol	Joback Method
hf	92.92	kJ/mol	Joback Method
hfl	-24.00	kJ/mol	NIST Webbook
hfus	15.47	kJ/mol	Joback Method
hvap	40.14	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.397		Crippen Method
mcvol	77.830	ml/mol	McGowan Method
pc	6113.06	kPa	Joback Method
tb	435.96	K	Joback Method
tc	686.19	K	Joback Method
tf	229.54	K	Joback Method
vc	0.280	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	95.12	J/mol×K	435.96	Joback Method
cpg	97.36	J/mol×K	477.67	Joback Method
cpg	99.24	J/mol×K	519.37	Joback Method
cpg	100.81	J/mol×K	561.08	Joback Method
cpg	102.10	J/mol×K	602.78	Joback Method
cpg	103.17	J/mol×K	644.49	Joback Method
cpg	104.04	J/mol×K	686.19	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72087913&Units=SI

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