Dichloromethanesulphonyl chloride

Other names: Dichloromethyl sulfonylchloride
Inchi: InChI=1S/CHCl3O2S/c2-1(3)7(4,5)6/h1H
InchiKey: ZTCPYHGKJGSSPD-UHFFFAOYSA-N
Formula: CHCl3O2S
SMILES: O=S(=O)(Cl)C(Cl)Cl
Mol. weight [g/mol]: 183.44

Physical Properties

Property code	Value	Unit	Source
gf	-549.23	kJ/mol	Joback Method
hf	-569.82	kJ/mol	Joback Method
hfus	18.79	kJ/mol	Joback Method
hvap	49.22	kJ/mol	Joback Method
log10ws	-1.63		Crippen Method
logp	1.316		Crippen Method
mcvol	89.760	ml/mol	McGowan Method
pc	6278.87	kPa	Joback Method
rinpol	970.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	970.00		NIST Webbook
tb	381.91	K	Joback Method
tc	577.35	K	Joback Method
tf	214.35	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	126.52	J/mol×K	381.91	Joback Method
cpg	130.37	J/mol×K	414.48	Joback Method
cpg	134.06	J/mol×K	447.06	Joback Method
cpg	137.59	J/mol×K	479.63	Joback Method
cpg	140.94	J/mol×K	512.20	Joback Method
cpg	144.11	J/mol×K	544.77	Joback Method

cpg	147.10	J/mol×K	577.35	Joback Method

Sources

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=U342592&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume