Chloromethanesulfonyl chloride

Other names:	Methanesulfonyl chloride, chloro- Chlorid kyseliny chlormethansulfonove Chlormethansulfochlorid Chlormethansulfonylchlorid chloromethanesulphonyl chloride
Inchi:	InChI=1S/CH2Cl2O2S/c2-1-6(3,4)5/h1H2
InchiKey:	KQDDQXNVESLJNO-UHFFFAOYSA-N
Formula:	CH2Cl2O2S
SMILES:	O=S(=O)(Cl)CCl
Mol. weight [g/mol]:	149.00
CAS:	3518-65-8

Physical Properties

Property code	Value	Unit	Source
gf	-534.86	kJ/mol	Joback Method
hf	-548.80	kJ/mol	Joback Method
hfus	18.12	kJ/mol	Joback Method
hvap	45.22	kJ/mol	Joback Method
log10ws	-0.87		Crippen Method
logp	0.751		Crippen Method
mcvol	77.520	ml/mol	McGowan Method
pc	6577.70	kPa	Joback Method
rinpol	904.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	910.00		NIST Webbook
tb	344.92	K	Joback Method
tc	526.50	K	Joback Method
tf	199.43	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	108.84	J/mol×K	344.92	Joback Method

cpg	112.61	J/mol×K	375.18	Joback Method
cpg	116.27	J/mol×K	405.45	Joback Method
cpg	119.83	J/mol×K	435.71	Joback Method
cpg	123.27	J/mol×K	465.97	Joback Method
cpg	126.58	J/mol×K	496.23	Joback Method
cpg	129.76	J/mol×K	526.50	Joback Method

Sources

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=C3518658&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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