Methanesulfonyl chloride

Other names:	Chloro methyl sulfone
	Mesyl chloride
	Methanesulfonic acid chloride
	Methanesulfuryl chloride
	Methanesulphonyl chloride
	Methyl sulfochloride
	Methylsulfonyl chloride
	CH3SO2Cl
	NSC 15039
Inchi:	InChI=1S/CH3ClO2S/c1-5(2,3)4/h1H3
InchiKey:	QARBMVPHQWIHKH-UHFFFAOYSA-N
Formula:	CH3ClO2S
SMILES:	CS(=O)(=O)Cl
Mol. weight [g/mol]:	114.55
CAS:	124-63-0

Physical Properties

Property code	Value	Unit	Source
gf	-522.93	kJ/mol	Joback Method
hf	-533.06	kJ/mol	Joback Method
hfus	13.92	kJ/mol	Joback Method
hvap	40.84	kJ/mol	Joback Method
ie	11.60	eV	NIST Webbook
ie	11.60	eV	NIST Webbook
ie	11.74	eV	NIST Webbook
log10ws	-0.22		Crippen Method
logp	0.185		Crippen Method
mcvol	65.280	ml/mol	McGowan Method
pc	6990.97	kPa	Joback Method
rinpol	774.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	778.00		NIST Webbook
rinpol	742.00		NIST Webbook
rinpol	742.00		NIST Webbook
ripol	1216.00		NIST Webbook
ripol	1216.00		NIST Webbook
tb	307.49	K	Joback Method

tc	478.52	K	Joback Method
tf	169.51	K	Joback Method
vc	0.267	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	90.74	J/mol×K	307.49	Joback Method
cpg	94.50	J/mol×K	336.00	Joback Method
cpg	98.20	J/mol×K	364.50	Joback Method
cpg	101.83	J/mol×K	393.01	Joback Method
cpg	105.38	J/mol×K	421.51	Joback Method
cpg	108.84	J/mol×K	450.02	Joback Method
cpg	112.21	J/mol×K	478.52	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=C124630&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
ie: Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume