Methoxycarbonylsulfenyl chloride

Other names:	Carbonothioic acid, anhydrosulfide with thiohypochlorous acid, methyl ester thiocarbonic acid, anhydrosulphide with methyl thiohypochlorite
Inchi:	InChI=1S/C2H3ClO2S/c1-5-2(4)6-3/h1H3
InchiKey:	TXJXPZVVSLAQOQ-UHFFFAOYSA-N
Formula:	C2H3ClO2S
SMILES:	COC(=O)SCl
Mol. weight [g/mol]:	126.56
CAS:	26555-40-8

Physical Properties

Property code	Value	Unit	Source
gf	-246.77	kJ/mol	Joback Method
hf	-303.28	kJ/mol	Joback Method
hfus	12.05	kJ/mol	Joback Method
hvap	40.40	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.640		Crippen Method
mcvol	75.070	ml/mol	McGowan Method
pc	5220.69	kPa	Joback Method
tb	427.66	K	Joback Method
tc	644.29	K	Joback Method
tf	248.78	K	Joback Method
vc	0.275	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	117.15	J/mol×K	427.66	Joback Method
cpg	121.47	J/mol×K	463.77	Joback Method
cpg	125.70	J/mol×K	499.87	Joback Method
cpg	129.84	J/mol×K	535.98	Joback Method
cpg	133.84	J/mol×K	572.08	Joback Method
cpg	137.70	J/mol×K	608.19	Joback Method
cpg	141.40	J/mol×K	644.29	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=C26555408&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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