CH3OC(O)SC2H5

Other names:	S-Ethyl O-methyl thiocarbonate
	Carbonothioic acid, S-ethyl, methyl ester
	C2H5S(OCH3)CO
Inchi:	InChI=1S/C4H8O2S/c1-3-7-4(5)6-2/h3H2,1-2H3
InchiKey:	VVIAWLIDZAXESO-UHFFFAOYSA-N
Formula:	C4H8O2S
SMILES:	CCSC(=O)OC
Mol. weight [g/mol]:	120.17
CAS:	38103-96-7

Physical Properties

Property code	Value	Unit	Source
affp	833.90	kJ/mol	NIST Webbook
basg	802.90	kJ/mol	NIST Webbook
gf	-218.00	kJ/mol	Joback Method
hf	-328.82	kJ/mol	Joback Method
hfus	13.03	kJ/mol	Joback Method
hvap	40.47	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.506		Crippen Method
mcvol	91.010	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
tb	435.99	K	Joback Method
tc	640.35	K	Joback Method
tf	241.40	K	Joback Method
vc	0.338	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.75	J/mol×K	435.99	Joback Method
cpg	175.63	J/mol×K	470.05	Joback Method
cpg	183.28	J/mol×K	504.11	Joback Method
cpg	190.68	J/mol×K	538.17	Joback Method

cpg	197.82	J/mol×K	572.23	Joback Method
cpg	204.68	J/mol×K	606.29	Joback Method
cpg	211.26	J/mol×K	640.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38103967&Units=SI
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

Legend

affp:	Proton affinity
basg:	Gas basicity
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