

(CH3O)2CS

Other names:	O,O-Dimethyl monothiocarbonate O,O'-Dimethyl thiocarbonate O,O'-Dimethyl monothiocarbonate
Inchi:	InChI=1S/C3H6O2S/c1-4-3(6)5-2/h1-2H3
InchiKey:	BJIKOZOULYUROB-UHFFFAOYSA-N
Formula:	C3H6O2S
SMILES:	COC(=S)OC
Mol. weight [g/mol]:	106.14
CAS:	1115-13-5

Physical Properties

Property code	Value	Unit	Source
gf	-118.56	kJ/mol	Joback Method
hf	-223.19	kJ/mol	Joback Method
hfus	10.51	kJ/mol	Joback Method
hvap	33.82	kJ/mol	Joback Method
ie	8.99	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
log10ws	-0.60		Crippen Method
logp	0.564		Crippen Method
mcvol	76.920	ml/mol	McGowan Method
pc	4769.39	kPa	Joback Method
tb	382.92	K	Joback Method
tc	580.96	K	Joback Method
tf	202.30	K	Joback Method
vc	0.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.21	J/mol×K	382.92	Joback Method
cpg	135.06	J/mol×K	415.93	Joback Method
cpg	140.68	J/mol×K	448.93	Joback Method
cpg	146.09	J/mol×K	481.94	Joback Method

cpg	151.29	J/mol×K	514.95	Joback Method
cpg	156.27	J/mol×K	547.95	Joback Method
cpg	161.05	J/mol×K	580.96	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=C1115135&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
ie:	Ionization energy
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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