O,O'-Dimethyl thiocarbonate

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]:	106.15

Physical Properties

Property code	Value	Unit	Source
hfus	10.51	kJ/mol	Joback Method
ie	8.70	eV	NIST Webbook
ie	8.99	eV	NIST Webbook
logp	0.564		Crippen Method
mcvol	76.920	ml/mol	McGowan 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

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1115135&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume