

Carbonodithioic acid, S,S-dimethyl ester

Other names:	Carbonic acid, dithio-, S,S-dimethyl ester S,S-Dimethyl dithiocarbonate
Inchi:	InChI=1S/C3H6OS2/c1-5-3(4)6-2/h1-2H3
InchiKey:	IUXMJLLWUTWQFX-UHFFFAOYSA-N
Formula:	C3H6OS2
SMILES:	CSC(=O)SC
Mol. weight [g/mol]:	122.21
CAS:	868-84-8

Physical Properties

Property code	Value	Unit	Source
gf	-88.30	kJ/mol	Joback Method
hf	-134.09	kJ/mol	Joback Method
hfus	13.38	kJ/mol	Joback Method
hvap	42.65	kJ/mol	Joback Method
log10ws	-1.60		Crippen Method
logp	1.832		Crippen Method
mvol	87.400	ml/mol	McGowan Method
pc	5037.07	kPa	Joback Method
tb	459.47	K	Joback Method
tc	693.28	K	Joback Method
tf	242.30	K	Joback Method
vc	0.318	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.05	J/molxK	459.47	Joback Method
cpg	156.21	J/molxK	498.44	Joback Method
cpg	163.06	J/molxK	537.41	Joback Method
cpg	169.60	J/molxK	576.37	Joback Method
cpg	175.80	J/molxK	615.34	Joback Method
cpg	181.66	J/molxK	654.31	Joback Method
cpg	187.16	J/molxK	693.28	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=C868848&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
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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