

Dithio bis(thionoformic acid), diisopropyl ester

Other names:	bis(isopropyl) thioperoxydicarbonate
Inchi:	InChI=1S/C8H14O2S4/c1-5(2)9-7(11)13-14-8(12)10-6(3)4/h5-6H,1-4H3
InchiKey:	ZWWQICJTBOCQLA-UHFFFAOYSA-N
Formula:	C8H14O2S4
SMILES:	CC(C)OC(=S)SSC(=S)OC(C)C
Mol. weight [g/mol]:	270.46
CAS:	105-65-7

Physical Properties

Property code	Value	Unit	Source
gf	101.96	kJ/mol	Joback Method
hf	-106.71	kJ/mol	Joback Method
hfus	29.27	kJ/mol	Joback Method
hvap	64.54	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	3.788		Crippen Method
mcvol	192.120	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
tb	704.04	K	Joback Method
tc	959.89	K	Joback Method
tf	331.72	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	446.72	J/molxK	704.04	Joback Method
cpg	458.62	J/molxK	746.68	Joback Method
cpg	469.64	J/molxK	789.32	Joback Method
cpg	479.83	J/molxK	831.97	Joback Method
cpg	489.26	J/molxK	874.61	Joback Method
cpg	497.97	J/molxK	917.25	Joback Method
cpg	506.05	J/molxK	959.89	Joback Method

Sources

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=C105657&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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