

Propanoic acid, 3,3'-thiobis-, dimethyl ester

Other names:	Dimethyl 3,3'-thiodipropionate «beta», «beta»'-Dicarbomethoxydiethyl sulfide Bis(2-methoxycarbonylethyl)sulfide Dimethyl thiodipropionate Propionic acid, 3,3'-thiodi-, dimethyl ester Thiodipropionic acid dimethyl ester 3,3'-Thiobis(methyl propionate) dimethyl 3,3'-thiobispropionate
Inchi:	InChI=1S/C8H14O4S/c1-11-7(9)3-5-13-6-4-8(10)12-2/h3-6H2,1-2H3
InchiKey:	MYWWWNVEZBAKHR-UHFFFAOYSA-N
Formula:	C8H14O4S
SMILES:	COC(=O)CCSCCC(=O)OC
Mol. weight [g/mol]:	206.26
CAS:	4131-74-2

Physical Properties

Property code	Value	Unit	Source
gf	-418.24	kJ/mol	Joback Method
hf	-656.18	kJ/mol	Joback Method
hfus	26.18	kJ/mol	Joback Method
hvap	58.53	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	0.846		Crippen Method
mcvol	154.810	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
tb	603.80	K	Joback Method
tc	804.36	K	Joback Method
tf	358.64	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.17	J/molxK	603.80	Joback Method

cpg	384.03	J/mol×K	637.23	Joback Method
cpg	395.33	J/mol×K	670.65	Joback Method
cpg	406.06	J/mol×K	704.08	Joback Method
cpg	416.21	J/mol×K	737.51	Joback Method
cpg	425.75	J/mol×K	770.94	Joback Method
cpg	434.68	J/mol×K	804.36	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	421.20	K	2.40	NIST Webbook

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=C4131742&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point

vc: Critical Volume

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