

Thiodipropionic acid

Other names:	Propanoic acid, 3,3'-thiobis- Propionic acid, 3,3'-thiodi- «beta», «beta»'-Thiodipropionic acid Diethyl sulfide 2,2'-dicarboxylic acid Thiodihydracrylic acid Tyox A TDPA 3,3'-Thiodipropionic acid 4-Thiaheptanedioic acid 3,3'-Thiodipropanoic acid Bis(2-carboxyethyl) sulfide Kyselina «beta», «beta»'-thiodipropionova Sulfide, bis(2-carboxyethyl) Kyselina 3,3-thiodipropionova 3,3'-Thiobis-propanoic acid NSC 8166
Inchi:	InChI=1S/C6H10O4S/c7-5(8)1-3-11-4-2-6(9)10/h1-4H2,(H,7,8)(H,9,10)
InchiKey:	ODJQKYXPKWQWNK-UHFFFAOYSA-N
Formula:	C6H10O4S
SMILES:	O=C(O)CCSCCC(=O)O
Mol. weight [g/mol]:	178.21
CAS:	111-17-1

Physical Properties

Property code	Value	Unit	Source
gf	-498.72	kJ/mol	Joback Method
hf	-654.92	kJ/mol	Joback Method
hfus	26.80	kJ/mol	Joback Method
hvap	82.62	kJ/mol	Joback Method
log10ws	-0.42		Crippen Method
logp	0.669		Crippen Method
mcvol	126.630	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
tb	697.56	K	Joback Method
tc	885.64	K	Joback Method
tf	413.28	K	Joback Method
vc	0.475	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.57	J/mol×K	697.56	Joback Method
cpg	326.61	J/mol×K	728.91	Joback Method
cpg	333.23	J/mol×K	760.25	Joback Method
cpg	339.45	J/mol×K	791.60	Joback Method
cpg	345.26	J/mol×K	822.95	Joback Method
cpg	350.68	J/mol×K	854.29	Joback Method
cpg	355.71	J/mol×K	885.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111171&Units=SI
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

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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