Propanoic acid, 3,3'-thiobis-

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

Physical Properties

Property code	Value	Unit	Source
af	0.8392		Cheméo Relay (1.0)
hf	-792.75	kJ/mol	Cheméo Relay (1.0)
hfus	26.80	kJ/mol	Joback Method
hvap	120.10	kJ/mol	Cheméo Relay (1.0)
ie	9.55	eV	Cheméo Relay (1.0)
log10ws	-0.20		Cheméo Relay (1.0)
logp	0.669		Crippen Method
mcvol	126.630	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
tb	568.71	K	Cheméo Relay (1.0)
tc	811.61	K	Cheméo Relay (1.0)
tf	387.28	K	Cheméo Relay (1.0)
vc	0.432	m3/kmol	Cheméo Relay (1.0)

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111171&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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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