Propanoic acid, 3,3'-dithiobis-

Other names:	3,3'-Dithiobis(dipropionic acid)
	3,3'-Dithiodipropionic acid
	3,3'-dithiobispropionic acid
	3-(2-carboxyethyldisulfanyl)propanoic acid
	Bis(2-carboxyethyl)disulfide
	Dithiodipropionic acid
	Propionic acid, 3,3'-dithiodi-
	«beta»,«beta»'-Dithiodipropionic acid
	Â«betaÂ»,Â«betaÂ»'-Dithiodipropionic acid
Inchi:	InChI=1S/C6H10O4S2/c7-5(8)1-3-11-12-4-2-6(9)10/h1-4H2,(H,7,8)(H,9,10)
InchiKey:	YCLSOMLVSHPPFV-UHFFFAOYSA-N
Formula:	C6H10O4S2
SMILES:	O=C(O)CCSSCCC(=O)O
Mol. weight [g/mol]:	210.27
CAS:	1119-62-6

Physical Properties

Property code	Value	Unit	Source
gf	-465.60	kJ/mol	Joback Method
hf	-613.05	kJ/mol	Joback Method
hfus	30.93	kJ/mol	Joback Method
hvap	89.43	kJ/mol	Joback Method
log10ws	-0.19		Aqueous Solubility Prediction Method
logp	1.317		Crippen Method
mcvol	142.980	ml/mol	McGowan Method
pc	4756.24	kPa	Joback Method
tb	766.34	K	Joback Method
tc	968.14	K	Joback Method
tf	447.68	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	360.96	J/mol×K	766.34	Joback Method
cpg	367.75	J/mol×K	799.97	Joback Method
cpg	374.02	J/mol×K	833.61	Joback Method
cpg	379.77	J/mol×K	867.24	Joback Method
cpg	385.00	J/mol×K	900.87	Joback Method
cpg	389.72	J/mol×K	934.51	Joback Method
cpg	393.92	J/mol×K	968.14	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1119626&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method: https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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