«beta»'-Dithiodilactic acid

Other names:	2-(1-hydroxy-1-oxopropan-2-yl)disulfanylpropanoic acid
	«alpha»,«alpha»'-Dithiodipropionic acid
	Â«alphaÂ»,Â«alphaÂ»'-Dithiodipropionic acid
Inchi:	InChI=1S/C6H10O4S2/c1-3(5(7)8)11-12-4(2)6(9)10/h3-4H,1-2H3,(H,7,8)(H,9,10)
InchiKey:	UTDRPUGFHHVEDG-UHFFFAOYSA-N
Formula:	C6H10O4S2
SMILES:	CC(SSC(C)C(=O)O)C(=O)O
Mol. weight [g/mol]:	210.27
CAS:	4775-93-3

Physical Properties

Property code	Value	Unit	Source
chs	-4028.40 ± 3.80	kJ/mol	NIST Webbook
gf	-470.48	kJ/mol	Joback Method
hf	-623.61	kJ/mol	Joback Method
hfus	23.88	kJ/mol	Joback Method
hvap	88.66	kJ/mol	Joback Method
log10ws	-0.61		Aqueous Solubility Prediction Method
logp	1.314		Crippen Method
mcvol	142.980	ml/mol	McGowan Method
pc	4862.97	kPa	Joback Method
ss	274.10	J/mol×K	NIST Webbook
tb	765.46	K	Joback Method
tc	973.00	K	Joback Method
tf	417.68	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.52	J/mol×K	938.41	Joback Method
cpg	362.27	J/mol×K	765.46	Joback Method
cpg	369.26	J/mol×K	800.05	Joback Method

cpg	375.68	J/mol×K	834.64	Joback Method
cpg	381.53	J/mol×K	869.23	Joback Method
cpg	386.81	J/mol×K	903.82	Joback Method
cpg	395.67	J/mol×K	973.00	Joback Method
cps	239.30	J/mol×K	296.80	NIST Webbook

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4775933&Units=SI

Legend

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

cps: Solid phase 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

ss: Solid phase molar entropy at standard conditions

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume