

2,2'-Thiodisuccinic acid

Other names:	Thiodisuccinic acid Butanedioic acid, 2,2'-thiobis-
Inchi:	InChI=1S/C8H10O8S/c9-5(10)1-3(7(13)14)17-4(8(15)16)2-6(11)12/h3-4H,1-2H2,(H,9,10)
InchiKey:	SASYRHXXVHLPMQD-UHFFFAOYSA-N
Formula:	C8H10O8S
SMILES:	O=C(O)CC(SC(CC(=O)O)C(=O)O)C(=O)O
Mol. weight [g/mol]:	266.23
CAS:	4917-76-4

Physical Properties

Property code	Value	Unit	Source
gf	-1018.24	kJ/mol	Joback Method
hf	-1236.38	kJ/mol	Joback Method
hfus	36.31	kJ/mol	Joback Method
hvap	133.14	kJ/mol	Joback Method
log10ws	0.32		Crippen Method
logp	-0.425		Crippen Method
mvol	169.690	ml/mol	McGowan Method
pc	5627.81	kPa	Joback Method
tb	1034.54	K	Joback Method
tc	1270.21	K	Joback Method
tf	627.32	K	Joback Method
vc	0.625	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.35	J/molxK	1034.54	Joback Method
cpg	498.04	J/molxK	1073.82	Joback Method
cpg	501.01	J/molxK	1113.10	Joback Method
cpg	503.27	J/molxK	1152.38	Joback Method
cpg	504.84	J/molxK	1191.65	Joback Method
cpg	505.75	J/molxK	1230.93	Joback Method
cpg	506.01	J/molxK	1270.21	Joback Method

Sources

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=C4917764&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	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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