Methanesulfonothioic acid, S,S'-1,4-butanediyl ester

Other names: 1,4-Butanediol, S-dimethanethiosulfonate
Inchi: InChI=1S/C6H14O4S4/c1-13(7,8)11-5-3-4-6-12-14(2,9)10/h3-6H2,1-2H3
InchiKey: VIISOSSRZYEECK-UHFFFAOYSA-N
Formula: C6H14O4S4
SMILES: CS(=O)(=O)SCCCCSS(C)(=O)=O
Mol. weight [g/mol]: 278.43
CAS: 55-99-2

Physical Properties

Property code	Value	Unit	Source
gf	-871.20	kJ/mol	Joback Method
hf	-990.13	kJ/mol	Joback Method
hfus	42.31	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	-1.75		Crippen Method
logp	1.152		Crippen Method
mcvol	184.280	ml/mol	McGowan Method
pc	4756.24	kPa	Joback Method
tb	569.80	K	Joback Method
tc	768.15	K	Joback Method
tf	303.30	K	Joback Method
vc	0.732	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.97	J/mol×K	569.80	Joback Method
cpg	423.12	J/mol×K	602.86	Joback Method
cpg	435.60	J/mol×K	635.92	Joback Method
cpg	447.36	J/mol×K	668.97	Joback Method
cpg	458.40	J/mol×K	702.03	Joback Method
cpg	468.68	J/mol×K	735.09	Joback Method
cpg	478.17	J/mol×K	768.15	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=C55992&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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