3,5-Dithiahexanol 5,5-dioxide

Other names: 2-(((Methylsulfonyl)methyl)thio)ethanol
Inchi: InChI=1S/C4H10O3S2/c1-9(6,7)4-8-3-2-5/h5H,2-4H2,1H3
InchiKey: IHCZCIDTAQHMPU-UHFFFAOYSA-N
Formula: C4H10O3S2
SMILES: CS(=O)(=O)CSCCO
Mol. weight [g/mol]: 170.25
CAS: 68483-74-9

Physical Properties

Property code	Value	Unit	Source
gf	-589.44	kJ/mol	Joback Method
hf	-689.60	kJ/mol	Joback Method
hfus	25.71	kJ/mol	Joback Method
hvap	66.63	kJ/mol	Joback Method
log10ws	0.03		Crippen Method
logp	-0.286		Crippen Method
mcvol	117.530	ml/mol	McGowan Method
pc	5585.83	kPa	Joback Method
rinpol	1542.70		NIST Webbook
rinpol	1542.70		NIST Webbook
tb	499.66	K	Joback Method
tc	679.38	K	Joback Method
tf	268.62	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.01	J/mol×K	499.66	Joback Method
cpg	253.65	J/mol×K	529.61	Joback Method
cpg	261.95	J/mol×K	559.57	Joback Method
cpg	269.91	J/mol×K	589.52	Joback Method
cpg	277.51	J/mol×K	619.47	Joback Method
cpg	284.75	J/mol×K	649.42	Joback Method

cpg	291.62	J/mol×K	679.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68483749&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume