

N,N'-Bis(2-hydroxyethyl)dithiooxamide

Other names:	Ethanedithioamide, N,N'-bis(2-hydroxyethyl)- Oxamide, N,N'-bis(2-hydroxyethyl)dithio- USAF mk-5 N,N'-Bis(2-hydroxyethyl)dithiooxamide
Inchi:	InChI=1S/C6H12N2O2S2/c9-3-1-7-5(11)6(12)8-2-4-10/h9-10H,1-4H2,(H,7,11)(H,8,12)
InchiKey:	POHRRIXAXBVBFW-UHFFFAOYSA-N
Formula:	C6H12N2O2S2
SMILES:	OCCNC(=S)C(=S)NCCO
Mol. weight [g/mol]:	208.30
CAS:	120-86-5

Physical Properties

Property code	Value	Unit	Source
gf	138.90	kJ/mol	Joback Method
hf	-71.69	kJ/mol	Joback Method
hfus	38.88	kJ/mol	Joback Method
hvap	88.64	kJ/mol	Joback Method
log10ws	-0.94		Crippen Method
logp	-1.195		Crippen Method
mcvol	151.200	ml/mol	McGowan Method
pc	5102.04	kPa	Joback Method
tb	761.46	K	Joback Method
tc	959.56	K	Joback Method
tf	452.88	K	Joback Method
vc	0.551	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.04	J/molxK	761.46	Joback Method
cpg	391.79	J/molxK	794.48	Joback Method
cpg	398.24	J/molxK	827.49	Joback Method
cpg	404.46	J/molxK	860.51	Joback Method
cpg	410.53	J/molxK	893.53	Joback Method

cpg	416.50	J/mol×K	926.54	Joback Method
cpg	422.44	J/mol×K	959.56	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C120865&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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