

Ethanol, 2,2'-[1,2-ethanediy]bis(thio)]bis-

Other names:	Ethanol, 2,2'-(ethylenedithio)di- Di(«beta»-Hydroxyethyl) ethylene disulfide Ethylenedithioethanol 1,10-Dioxa-4,7-dithiadecane 1,2-Bis(«beta»-hydroxyethylthio)ethane 1,2-Bis(2-hydroxyethylthio)ethane 1,8-Dihydroxy-3,6-dithiaoctane 2,2'-[1,2-Ethanediy]bis(thio)]bisethanol 3,6-Dithia-1,8-octanediol 1,2-Bis(beta-hydroxyethylthio)ethane 1,8-Dihydroxy-3,6-dithiooctane 1,8-Dihydroxy-3,6-octanedithione 2,2'-(Ethylenedithio)diethanol 3,6-Dithiaoctan-1,8-diol
Inchi:	InChI=1S/C6H14O2S2/c7-1-3-9-5-6-10-4-2-8/h7-8H,1-6H2
InchiKey:	PDHFSBFXZGYBIP-UHFFFAOYSA-N
Formula:	C6H14O2S2
SMILES:	OCCSCCSCCO
Mol. weight [g/mol]:	182.30
CAS:	5244-34-8

Physical Properties

Property code	Value	Unit	Source
gf	-207.76	kJ/mol	Joback Method
hf	-387.89	kJ/mol	Joback Method
hfus	27.73	kJ/mol	Joback Method
hvap	75.94	kJ/mol	Joback Method
log10ws	-0.63		Crippen Method
logp	0.437		Crippen Method
mcvol	139.840	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	1703.00		NIST Webbook
rinpol	1703.00		NIST Webbook
tb	658.60	K	Joback Method
tc	846.58	K	Joback Method
tf	347.82	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.79	J/mol×K	658.60	Joback Method
cpg	355.64	J/mol×K	689.93	Joback Method
cpg	364.04	J/mol×K	721.26	Joback Method
cpg	371.98	J/mol×K	752.59	Joback Method
cpg	379.48	J/mol×K	783.92	Joback Method
cpg	386.53	J/mol×K	815.25	Joback Method
cpg	393.15	J/mol×K	846.58	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	443.20	K	0.07	NIST Webbook

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=C5244348&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
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
mcpvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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