

Ethanethiol, 2,2'-thiobis-

Other names:	Ethanethiol, 2,2'-thiodi- Bis(mercaptoethyl) sulfide Bis(2-mercaptoethyl) sulfide TDT 1-Mercapto-2-(mercaptoethylthio)ethane 2-Mercaptoethyl sulfide 2,2'-Dimercaptodiethyl sulfide 2,2'-Thiodiethanethiol 3-Thia-1,5-pentanedithiol «beta», «beta»'-Dimercaptoethyl sulfide Bis(«beta»-mercaptoethyl) sulfide 1,5-Dimercapto-3-thiapentane Bis(2-sulfanylethyl) sulfide NSC 4766
Inchi:	InChI=1S/C4H10S3/c5-1-3-7-4-2-6/h5-6H,1-4H2
InchiKey:	KSJBMDCFYZKAFH-UHFFFAOYSA-N
Formula:	C4H10S3
SMILES:	SCCSCCS
Mol. weight [g/mol]:	154.32
CAS:	3570-55-6

Physical Properties

Property code	Value	Unit	Source
gf	74.70	kJ/mol	Joback Method
hf	-7.06	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	44.79	kJ/mol	Joback Method
log10ws	-1.52		Crippen Method
logp	1.579		Crippen Method
mvol	116.270	ml/mol	McGowan Method
pc	4710.65	kPa	Joback Method
tb	485.42	K	Joback Method
tc	729.25	K	Joback Method
tf	242.16	K	Joback Method
vc	0.421	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.26	J/molxK	485.42	Joback Method
cpg	224.31	J/molxK	526.06	Joback Method
cpg	233.82	J/molxK	566.70	Joback Method
cpg	242.78	J/molxK	607.34	Joback Method
cpg	251.21	J/molxK	647.97	Joback Method
cpg	259.11	J/molxK	688.61	Joback Method
cpg	266.49	J/molxK	729.25	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.70	K	1.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3570556&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
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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