

2,2'-DITHIODIETHANOL

Other names:	Ethanol, 2,2'-dithiodi- Bis(2-hydroxyethyl) disulfide Diethanol disulfide Dithiodiglycol Hydroxyethyl disulfide 2-Hydroxyethanedisulfide 2-Hydroxyethyl disulfide 2,2'-Dithiodiethanol 3,4-Dithia-1,6-hexanediol USAF TH-9 2,2'-Dithiobisethanol 2-Mercaptoethanol disulfide NSC 33920 «beta»-Hydroxyethyl disulfide
Inchi:	InChI=1S/C4H10O2S2/c5-1-3-7-8-4-2-6/h5-6H,1-4H2
InchiKey:	KYNFOMQIXZUKRK-UHFFFAOYSA-N
Formula:	C4H10O2S2
SMILES:	OCCSSCCO
Mol. weight [g/mol]:	154.26

Physical Properties

Property code	Value	Unit	Source
hfus	22.55	kJ/mol	Joback Method
logp	0.352		Crippen Method
mcvol	111.660	ml/mol	McGowan Method
rinpol	1425.00		NIST Webbook
tb	585.83	K	Cheméo Relay (1.0)
tf	271.71	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.80	J/mol×K	612.84	Joback Method
cpg	260.91	J/mol×K	644.81	Joback Method

cpg	267.67	J/mol×K	676.77	Joback Method
cpg	274.07	J/mol×K	708.74	Joback Method
cpg	280.13	J/mol×K	740.71	Joback Method
cpg	285.83	J/mol×K	772.68	Joback Method
cpg	291.17	J/mol×K	804.64	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	433.70	K	0.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1892291&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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