

Thiodiglycol

Other names:	.beta.,.beta.'-dihydroxydiethyl sulfide .beta.-thiodiglycol 2,2'-Thiobis[ethanol] 2,2'-Thiodiglycol 2,2'-thiodiethanol 2,2-Thiodiethanol 3-Thiapentane-1,5-diol Bis(2-hydroxyethyl) sulphide Bis(2-hydroxyethyl) thioether Bis(2-hydroxyethyl)sulfide Bis(b-hydroxyethyl) sulfide Bis(«beta»-hydroxyethyl) sulfide Di(2-hydroxyethyl) sulfide Diethanol sulfide Dihydroxyethyl sulfide Ethanol, 2,2'-thiodi- Glyecine A Kromfax solvent NSC 6289 Sulfide, bis(2-hydroxyethyl) Tedegyl Thiodiethanol bis(2-hydroxyethyl) sulfide ethanol, 2,2'-thiobis- thiodiethylene glycol «beta»,«beta»'-Dihydroxydiethyl sulfide «beta»,«beta»'-Dihydroxyethyl sulfide «beta»-Bis(hydroxyethyl) sulfide «beta»-Hydroxyethyl sulfide «beta»-Thiodiglycol
Inchi:	InChI=1S/C4H10O2S/c5-1-3-7-4-2-6/h5-6H,1-4H2
InchiKey:	YODZTKMDCQEPHD-UHFFFAOYSA-N
Formula:	C4H10O2S
SMILES:	OCCSCCO
Mol. weight [g/mol]:	122.19
CAS:	111-48-8

Physical Properties

Property code	Value	Unit	Source
gf	-257.72	kJ/mol	Joback Method
hf	-388.48	kJ/mol	Joback Method
hfus	18.42	kJ/mol	Joback Method
hvap	64.67	kJ/mol	Joback Method
log10ws	0.09		Crippen Method
logp	-0.296		Crippen Method
mcvol	95.310	ml/mol	McGowan Method
pc	5094.76	kPa	Joback Method
rinpol	1184.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1184.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1130.90		NIST Webbook
rinpol	1181.50		NIST Webbook
rinpol	1181.50		NIST Webbook
ripol	2423.00		NIST Webbook
ripol	2422.60		NIST Webbook
ripol	2393.00		NIST Webbook
ripol	2382.00		NIST Webbook
ripol	2423.00		NIST Webbook
ripol	2422.60		NIST Webbook
ripol	2351.90		NIST Webbook
ripol	2382.00		NIST Webbook
tb	556.15	K	NIST Webbook
tc	719.76	K	Joback Method
tf	263.15	K	NIST Webbook
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.10	J/mol×K	719.76	Joback Method

cpg	213.30	J/mol×K	544.06	Joback Method
cpg	244.65	J/mol×K	690.47	Joback Method
cpg	238.93	J/mol×K	661.19	Joback Method
cpg	232.94	J/mol×K	631.91	Joback Method
cpg	226.67	J/mol×K	602.63	Joback Method
cpg	220.13	J/mol×K	573.34	Joback Method
hvapt	28.30	kJ/mol	436.50	NIST Webbook
hvapt	27.10	kJ/mol	425.50	NIST Webbook
pvap	3.67e-04	kPa	313.15	Vapor Pressure of Thiodiglycol
pvap	2.00e-04	kPa	308.15	Vapor Pressure of Thiodiglycol
pvap	1.28e-04	kPa	303.15	Vapor Pressure of Thiodiglycol
pvap	6.53e-05	kPa	298.15	Vapor Pressure of Thiodiglycol
rhoI	1174.00	kg/m3	303.15	Experimental solubility of carbon dioxide and hydrogen sulfide in 2,2'-thiodiglycol
rhoI	1182.40	kg/m3	293.15	Experimental solubility of carbon dioxide and hydrogen sulfide in 2,2'-thiodiglycol
rhoI	1160.00	kg/m3	323.15	Experimental solubility of carbon dioxide and hydrogen sulfide in 2,2'-thiodiglycol
rhoI	1167.00	kg/m3	313.15	Experimental solubility of carbon dioxide and hydrogen sulfide in 2,2'-thiodiglycol
rhoI	1145.00	kg/m3	343.15	Experimental solubility of carbon dioxide and hydrogen sulfide in 2,2'-thiodiglycol
rhoI	1138.00	kg/m3	353.15	Experimental solubility of carbon dioxide and hydrogen sulfide in 2,2'-thiodiglycol

rhoI	1152.00	kg/m3	333.15	Experimental solubility of carbon dioxide and hydrogen sulfide in 2,2'-thiodiglycol
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Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	438.20	K	2.70	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111488&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Experimental solubility of carbon dioxide and hydrogen sulfide in 2,2'-thiodiglycol:	https://www.doi.org/10.1016/j.jct.2019.02.024
Vapor Pressure:	https://www.doi.org/10.1021/je400978j
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoI:	Liquid Density
rinpol:	Non-polar retention indices

ripol:	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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