

# Monothioglycerol

<b>Other names:</b>	3-Mercapto-1,2-propanediol 1-Thioglycerol «alpha»-Thioglycerol Thioglycerol 1,2-Propanediol, 3-mercapto- «alpha»-Monothioglycerol «alpha»-Thiolglycerol Glycerol-1-thiol Glycerol, 1-thio- Thioglycerin Thioglycerine Thiovanol USAF CB-37 USAF B-40 1-Mercapto-2,3-propanediol 1-Mercaptoglycerol 1-Monothioglycerol 1-Thio-2,3-propanediol 2,3-Dihydroxypropanethiol Monothioglycerin 3-Mercaptopropane-1,2-diol NSC 5370
<b>Inchi:</b>	InChI=1S/C3H8O2S/c4-1-3(5)2-6/h3-6H,1-2H2
<b>InchiKey:</b>	PJUIMOJAAPLTRJ-UHFFFAOYSA-N
<b>Formula:</b>	C3H8O2S
<b>SMILES:</b>	OCC(O)CS
<b>Mol. weight [g/mol]:</b>	108.16
<b>CAS:</b>	96-27-5

## Physical Properties

Property code	Value	Unit	Source
gf	-272.31	kJ/mol	Joback Method
hf	-376.51	kJ/mol	Joback Method
hfus	12.22	kJ/mol	Joback Method
hvap	61.98	kJ/mol	Joback Method
log10ws	0.21		Crippen Method

logp	-0.731		Crippen Method
mvol	81.220	ml/mol	McGowan Method
pc	6400.00	kPa	Joback Method
tb	514.82	K	Joback Method
tc	695.63	K	Joback Method
tf	266.67	K	Joback Method
vc	0.289	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	171.60	J/mol×K	514.82	Joback Method
cpg	177.39	J/mol×K	544.96	Joback Method
cpg	182.92	J/mol×K	575.09	Joback Method
cpg	188.19	J/mol×K	605.23	Joback Method
cpg	193.21	J/mol×K	635.36	Joback Method
cpg	197.99	J/mol×K	665.50	Joback Method
cpg	202.54	J/mol×K	695.63	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	391.20	K	0.70	NIST Webbook

## Sources

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Joback Method:**

[https://en.wikipedia.org/wiki/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=C96275&Units=SI>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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