

# 3,3'-Thiodipropanol

<b>Other names:</b>	1-Propanol, 3,3'-thiobis-Thiodipropanol 3,3'-thiodipropan-1-ol
<b>Inchi:</b>	InChI=1S/C6H14O2S/c7-3-1-5-9-6-2-4-8/h7-8H,1-6H2
<b>InchiKey:</b>	QRQVZZMTKYXEKC-UHFFFAOYSA-N
<b>Formula:</b>	C6H14O2S
<b>SMILES:</b>	OCCSCCCO
<b>Mol. weight [g/mol]:</b>	150.24
<b>CAS:</b>	10595-09-2

## Physical Properties

Property code	Value	Unit	Source
gf	-240.88	kJ/mol	Joback Method
hf	-429.76	kJ/mol	Joback Method
hfus	23.60	kJ/mol	Joback Method
hvap	69.12	kJ/mol	Joback Method
log10ws	-0.74		Crippen Method
logp	0.484		Crippen Method
mcvol	123.490	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
tb	589.82	K	Joback Method
tc	762.90	K	Joback Method
tf	313.42	K	Joback Method
vc	0.464	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.13	J/molxK	589.82	Joback Method
cpg	309.86	J/molxK	618.67	Joback Method
cpg	318.22	J/molxK	647.51	Joback Method
cpg	326.21	J/molxK	676.36	Joback Method
cpg	333.84	J/molxK	705.21	Joback Method
cpg	341.11	J/molxK	734.06	Joback Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C10595092&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10595092&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## 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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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