

# 1-Propanol, 2,3-bis-(methylthio)

<b>Inchi:</b>	InChI=1S/C5H12OS2/c1-7-4-5(3-6)8-2/h5-6H,3-4H2,1-2H3
<b>InchiKey:</b>	NWIGMDHZYOQICC-UHFFFAOYSA-N
<b>Formula:</b>	C5H12OS2
<b>SMILES:</b>	CSCC(CO)SC
<b>Mol. weight [g/mol]:</b>	152.28

## Physical Properties

Property code	Value	Unit	Source
gf	-81.80	kJ/mol	Joback Method
hf	-220.30	kJ/mol	Joback Method
hfus	17.53	kJ/mol	Joback Method
hvap	56.65	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	1.073		Crippen Method
mcvol	119.880	ml/mol	McGowan Method
pc	4088.15	kPa	Joback Method
rinsol	1236.00		NIST Webbook
tb	543.10	K	Joback Method
tc	748.61	K	Joback Method
tf	260.73	K	Joback Method
vc	0.436	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.77	J/mol×K	543.10	Joback Method
cpg	267.50	J/mol×K	577.35	Joback Method
cpg	276.77	J/mol×K	611.60	Joback Method
cpg	285.57	J/mol×K	645.85	Joback Method
cpg	293.92	J/mol×K	680.10	Joback Method
cpg	301.80	J/mol×K	714.36	Joback Method
cpg	309.22	J/mol×K	748.61	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R121603&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R121603&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<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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