

# 3-mercaptononanol

<b>Inchi:</b>	InChI=1S/C9H20OS/c1-2-3-4-5-6-9(11)7-8-10/h9-11H,2-8H2,1H3
<b>InchiKey:</b>	AGWMDKCBKRLFRA-UHFFFAOYSA-N
<b>Formula:</b>	C9H20OS
<b>SMILES:</b>	CCCCCCC(S)CCO
<b>Mol. weight [g/mol]:</b>	176.32

## Physical Properties

Property code	Value	Unit	Source
gf	-84.97	kJ/mol	Joback Method
hf	-348.12	kJ/mol	Joback Method
hfus	23.67	kJ/mol	Joback Method
hvap	58.66	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	2.638		Crippen Method
mvol	159.890	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rmpol	1424.00		NIST Webbook
tb	559.92	K	Joback Method
tc	738.68	K	Joback Method
tf	273.47	K	Joback Method
vc	0.607	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.56	J/mol×K	559.92	Joback Method
cpg	400.55	J/mol×K	589.71	Joback Method
cpg	412.97	J/mol×K	619.51	Joback Method
cpg	424.82	J/mol×K	649.30	Joback Method
cpg	436.12	J/mol×K	679.09	Joback Method
cpg	446.91	J/mol×K	708.89	Joback Method
cpg	457.18	J/mol×K	738.68	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=R292047&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R292047&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.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>

# 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>rinpola:</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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