

# 2-Mercaptobenzyl alcohol

<b>Inchi:</b>	InChI=1S/C7H8OS/c8-5-6-3-1-2-4-7(6)9/h1-4,8-9H,5H2
<b>InchiKey:</b>	FYWFCRHZXORPFH-UHFFFAOYSA-N
<b>Formula:</b>	C7H8OS
<b>SMILES:</b>	OCc1ccccc1S
<b>Mol. weight [g/mol]:</b>	140.20
<b>CAS:</b>	4521-31-7

## Physical Properties

Property code	Value	Unit	Source
gf	3.41	kJ/mol	Joback Method
hf	-76.50	kJ/mol	Joback Method
hfus	15.67	kJ/mol	Joback Method
hvap	57.53	kJ/mol	Joback Method
log10ws	-2.13		Crippen Method
logp	1.468		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
pc	4973.33	kPa	Joback Method
tb	546.26	K	Joback Method
tc	768.10	K	Joback Method
tf	304.87	K	Joback Method
vc	0.393	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.09	J/molxK	546.26	Joback Method
cpg	232.47	J/molxK	583.23	Joback Method
cpg	241.25	J/molxK	620.21	Joback Method
cpg	249.45	J/molxK	657.18	Joback Method
cpg	257.11	J/molxK	694.15	Joback Method
cpg	264.24	J/molxK	731.13	Joback Method
cpg	270.88	J/molxK	768.10	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C4521317&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4521317&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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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