

# 2,2-Dimethyl heptanol

<b>Inchi:</b>	InChI=1S/C9H20O/c1-4-5-6-7-9(2,3)8-10/h10H,4-8H2,1-3H3
<b>InchiKey:</b>	WENIXZFPXMQPQQ-UHFFFAOYSA-N
<b>Formula:</b>	C9H20O
<b>SMILES:</b>	CCCCC(C)(C)CO
<b>Mol. weight [g/mol]:</b>	144.25

## Physical Properties

Property code	Value	Unit	Source
gf	-109.08	kJ/mol	Joback Method
hf	-390.07	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	51.01	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.585		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2574.11	kPa	Joback Method
tb	494.27	K	Joback Method
tc	662.00	K	Joback Method
tf	254.43	K	Joback Method
vc	0.547	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.27	J/molxK	494.27	Joback Method
cpg	398.12	J/molxK	634.04	Joback Method
cpg	387.08	J/molxK	606.09	Joback Method
cpg	375.49	J/molxK	578.13	Joback Method
cpg	363.35	J/molxK	550.18	Joback Method
cpg	350.61	J/molxK	522.22	Joback Method
cpg	408.65	J/molxK	662.00	Joback Method
dvisc	0.0001471	Paxs	494.27	Joback Method
dvisc	0.0002563	Paxs	454.30	Joback Method
dvisc	0.0004970	Paxs	414.32	Joback Method

dvisc	0.0011101	Paxs	374.35	Joback Method
dvisc	0.0030048	Paxs	334.38	Joback Method
dvisc	0.0106579	Paxs	294.40	Joback Method
dvisc	0.0562745	Paxs	254.43	Joback Method

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000989&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000989&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<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>hvac:</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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