

# 2,2,3-trimethylhexan-3-ol

Inchi:	InChI=1S/C9H20O/c1-6-7-9(5,10)8(2,3)4/h10H,6-7H2,1-5H3
InchiKey:	DHNHHYWBNQHGHN-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCCC(C)(O)C(C)(C)C
Mol. weight [g/mol]:	144.25
CAS:	5340-41-0

## Physical Properties

Property code	Value	Unit	Source
gf	-106.24	kJ/mol	Joback Method
hf	-398.82	kJ/mol	Joback Method
hfus	8.33	kJ/mol	Joback Method
hvap	49.72	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	2.584		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
tb	443.15 ± 4.00	K	NIST Webbook
tc	668.44	K	Joback Method
tf	256.85	K	Joback Method
vc	0.536	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	340.10	J/mol×K	491.04	Joback Method
cpg	354.48	J/mol×K	520.61	Joback Method
cpg	368.08	J/mol×K	550.17	Joback Method
cpg	380.92	J/mol×K	579.74	Joback Method
cpg	393.06	J/mol×K	609.30	Joback Method
cpg	404.53	J/mol×K	638.87	Joback Method
cpg	415.37	J/mol×K	668.44	Joback Method
dvisc	0.0749843	Paxs	256.85	Joback Method
dvisc	0.0133611	Paxs	295.88	Joback Method

dvisc	0.0035590	Paxs	334.91	Joback Method
dvisc	0.0012495	Paxs	373.94	Joback Method
dvisc	0.0005347	Paxs	412.98	Joback Method
dvisc	0.0002649	Paxs	452.01	Joback Method
dvisc	0.0001468	Paxs	491.04	Joback Method
hvapt	55.10	kJ/mol	392.00	NIST Webbook

## 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=C5340410&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5340410&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>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mvol:</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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