

# 3,4-Dimethyl-3-hexanol

<b>Other names:</b>	3-Hexanol, 3,4-dimethyl-
<b>Inchi:</b>	InChI=1S/C8H18O/c1-5-7(3)8(4,9)6-2/h7,9H,5-6H2,1-4H3
<b>InchiKey:</b>	FJXOYCIYKQJAAF-UHFFFAOYSA-N
<b>Formula:</b>	C8H18O
<b>SMILES:</b>	CCC(C)C(C)(O)CC
<b>Mol. weight [g/mol]:</b>	130.23
<b>CAS:</b>	19550-08-4

## Physical Properties

Property code	Value	Unit	Source
gf	-119.94	kJ/mol	Joback Method
hf	-374.71	kJ/mol	Joback Method
hfus	9.63	kJ/mol	Joback Method
hvap	48.40	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.194		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
ripol	1411.00		NIST Webbook
tb	434.15 ± 1.50	K	NIST Webbook
tc	643.32	K	Joback Method
tf	228.16	K	Joback Method
vc	0.485	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.99	J/mol×K	470.95	Joback Method
cpg	305.85	J/mol×K	499.68	Joback Method
cpg	318.10	J/mol×K	528.41	Joback Method
cpg	329.77	J/mol×K	557.13	Joback Method
cpg	340.87	J/mol×K	585.86	Joback Method
cpg	351.43	J/mol×K	614.59	Joback Method
cpg	361.48	J/mol×K	643.32	Joback Method

dvisc	0.1736472	Paxs	228.16	Joback Method
dvisc	0.0230030	Paxs	268.62	Joback Method
dvisc	0.0051732	Paxs	309.09	Joback Method
dvisc	0.0016435	Paxs	349.55	Joback Method
dvisc	0.0006624	Paxs	390.02	Joback Method
dvisc	0.0003167	Paxs	430.49	Joback Method
dvisc	0.0001719	Paxs	470.95	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.47217e+01
Coeff. B	-3.69423e+03
Coeff. C	-6.85070e+01
Temperature range (K), min.	324.44
Temperature range (K), max.	461.08

## 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=C19550084&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19550084&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>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>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log10 of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>p<sub>c</sub>:</b>	Critical Pressure
<b>p<sub>vap</sub>:</b>	Vapor pressure
<b>ri<sub>pol</sub>:</b>	Polar retention indices
<b>t<sub>b</sub>:</b>	Normal Boiling Point Temperature
<b>t<sub>c</sub>:</b>	Critical Temperature
<b>t<sub>f</sub>:</b>	Normal melting (fusion) point
<b>v<sub>c</sub>:</b>	Critical Volume

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