

# 3-Hexanol, 3,4-diethyl-

<b>Inchi:</b>	InChI=1S/C10H22O/c1-5-9(6-2)10(11,7-3)8-4/h9,11H,5-8H2,1-4H3
<b>InchiKey:</b>	WKHFIEUDEJOTPQ-UHFFFAOYSA-N
<b>Formula:</b>	C10H22O
<b>SMILES:</b>	CCC(CC)C(O)(CC)CC
<b>Mol. weight [g/mol]:</b>	158.28
<b>CAS:</b>	19398-78-8

## Physical Properties

Property code	Value	Unit	Source
gf	-103.10	kJ/mol	Joback Method
hf	-415.99	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	52.85	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.974		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
tb	516.71	K	Joback Method
tc	686.53	K	Joback Method
tf	250.70	K	Joback Method
vc	0.598	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.78	J/molxK	516.71	Joback Method
cpg	398.19	J/molxK	545.01	Joback Method
cpg	411.92	J/molxK	573.32	Joback Method
cpg	425.02	J/molxK	601.62	Joback Method
cpg	437.50	J/molxK	629.92	Joback Method
cpg	449.39	J/molxK	658.22	Joback Method
cpg	460.72	J/molxK	686.53	Joback Method
dvisc	0.0899105	Paxs	250.70	Joback Method
dvisc	0.0128169	Paxs	295.03	Joback Method

dvisc	0.0030395	Paxs	339.37	Joback Method
dvisc	0.0010052	Paxs	383.71	Joback Method
dvisc	0.0004181	Paxs	428.04	Joback Method
dvisc	0.0002050	Paxs	472.38	Joback Method
dvisc	0.0001136	Paxs	516.71	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=C19398788&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19398788&amp;Units=SI</a>
<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>

## 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>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</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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