

# 4-Hexyn-3-ol

<b>Inchi:</b>	InChI=1S/C6H10O/c1-3-5-6(7)4-2/h6-7H,4H2,1-2H3
<b>InchiKey:</b>	KARLLBDFLHNKBO-UHFFFAOYSA-N
<b>Formula:</b>	C6H10O
<b>SMILES:</b>	CC#CC(O)CC
<b>Mol. weight [g/mol]:</b>	98.14
<b>CAS:</b>	20739-59-7

## Physical Properties

Property code	Value	Unit	Source
gf	63.18	kJ/mol	Joback Method
hf	-52.38	kJ/mol	Joback Method
hfus	14.98	kJ/mol	Joback Method
hvap	47.39	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	0.781		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	4249.61	kPa	Joback Method
tb	437.42	K	Joback Method
tc	624.36	K	Joback Method
tf	309.30	K	Joback Method
vc	0.346	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.90	J/molxK	437.42	Joback Method
cpg	187.39	J/molxK	468.58	Joback Method
cpg	195.55	J/molxK	499.73	Joback Method
cpg	203.37	J/molxK	530.89	Joback Method
cpg	210.87	J/molxK	562.04	Joback Method
cpg	218.05	J/molxK	593.20	Joback Method
cpg	224.92	J/molxK	624.36	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.00	K	14.00	NIST Webbook

## Sources

Joback Method:	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C20739597&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C20739597&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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