

# 2-Hexyn-1-ol

<b>Other names:</b>	hex-2-yn-1-ol
<b>Inchi:</b>	InChI=1S/C6H10O/c1-2-3-4-5-6-7/h7H,2-3,6H2,1H3
<b>InchiKey:</b>	BTDWSZJDLLLLTMI-UHFFFAOYSA-N
<b>Formula:</b>	C6H10O
<b>SMILES:</b>	CCCC#CCO
<b>Mol. weight [g/mol]:</b>	98.14
<b>CAS:</b>	764-60-3

## Physical Properties

Property code	Value	Unit	Source
gf	65.62	kJ/mol	Joback Method
hf	-47.10	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	47.78	kJ/mol	Joback Method
log10ws	-1.39		Crippen Method
logp	0.782		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	4205.63	kPa	Joback Method
rinpol	820.50		NIST Webbook
rinpol	820.50		NIST Webbook
rinpol	847.00		NIST Webbook
ripol	1213.00		NIST Webbook
ripol	1213.00		NIST Webbook
ripol	1201.00		NIST Webbook
tb	437.86	K	Joback Method
tc	620.62	K	Joback Method
tf	324.30	K	Joback Method
vc	0.352	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	178.77	J/molxK	437.86	Joback Method
cpg	186.99	J/molxK	468.32	Joback Method

cpg	194.89	J/mol×K	498.78	Joback Method
cpg	202.48	J/mol×K	529.24	Joback Method
cpg	209.77	J/mol×K	559.70	Joback Method
cpg	216.77	J/mol×K	590.16	Joback Method
cpg	223.48	J/mol×K	620.62	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.00	K	7.10	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=C764603&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C764603&amp;Units=SI</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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature

**tf:** Normal melting (fusion) point

**vc:** Critical Volume

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