

# 4-Heptyn-2-ol

<b>Other names:</b>	hept-4-yn-2-ol
<b>Inchi:</b>	InChI=1S/C7H12O/c1-3-4-5-6-7(2)8/h7-8H,3,6H2,1-2H3
<b>InchiKey:</b>	CXVIEBMEWKSONY-UHFFFAOYSA-N
<b>Formula:</b>	C7H12O
<b>SMILES:</b>	CCC#CCC(C)O
<b>Mol. weight [g/mol]:</b>	112.17
<b>CAS:</b>	19781-81-8

## Physical Properties

Property code	Value	Unit	Source
gf	71.60	kJ/mol	Joback Method
hf	-73.02	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	49.62	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.171		Crippen Method
mcvol	106.760	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
tb	460.30	K	Joback Method
tc	645.47	K	Joback Method
tf	320.57	K	Joback Method
vc	0.403	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.62	J/mol×K	460.30	Joback Method
cpg	227.38	J/mol×K	491.16	Joback Method
cpg	236.73	J/mol×K	522.02	Joback Method
cpg	245.69	J/mol×K	552.89	Joback Method
cpg	254.28	J/mol×K	583.75	Joback Method
cpg	262.50	J/mol×K	614.61	Joback Method
cpg	270.36	J/mol×K	645.47	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.00	K	1.90	NIST Webbook

## Sources

<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=C19781818&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19781818&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>

## 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>hvp:</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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