

# 2-Hepten-4-ol

<b>Inchi:</b>	InChI=1S/C7H14O/c1-3-5-7(8)6-4-2/h3,5,7-8H,4,6H2,1-2H3/b5-3+
<b>InchiKey:</b>	DODCYMXUZOEQF-HWKANZROSA-N
<b>Formula:</b>	C7H14O
<b>SMILES:</b>	CC=CC(O)CCC
<b>Mol. weight [g/mol]:</b>	114.19
<b>CAS:</b>	4798-59-8

## Physical Properties

Property code	Value	Unit	Source
gf	-50.98	kJ/mol	Joback Method
hf	-228.10	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	47.42	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.723		Crippen Method
mcvol	111.060	ml/mol	McGowan Method
pc	3310.55	kPa	Joback Method
tb	426.00 ± 2.00	K	NIST Webbook
tc	626.76	K	Joback Method
tf	209.39	K	Joback Method
vc	0.420	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.62	J/mol×K	455.46	Joback Method
cpg	279.70	J/mol×K	598.21	Joback Method
cpg	270.95	J/mol×K	569.66	Joback Method
cpg	261.78	J/mol×K	541.11	Joback Method
cpg	252.19	J/mol×K	512.56	Joback Method
cpg	242.14	J/mol×K	484.01	Joback Method
cpg	288.05	J/mol×K	626.76	Joback Method
dvisc	0.0001634	Paxs	455.46	Joback Method
dvisc	0.0002941	Paxs	414.45	Joback Method

dvisc	0.0006019	Paxs	373.44	Joback Method
dvisc	0.0014702	Paxs	332.43	Joback Method
dvisc	0.0046173	Paxs	291.41	Joback Method
dvisc	0.0210963	Paxs	250.40	Joback Method
dvisc	0.1747804	Paxs	209.39	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=C4798598&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4798598&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>mcvol:</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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