

# 4-Hepten-3-ol, 4-methyl-

<b>Other names:</b>	4-Methyl-4-hepten-3-ol
<b>Inchi:</b>	InChI=1S/C8H16O/c1-4-6-7(3)8(9)5-2/h6,8-9H,4-5H2,1-3H3/b7-6+
<b>InchiKey:</b>	CVBRKUMJLIZGY-VOTSOKGWSA-N
<b>Formula:</b>	C8H16O
<b>SMILES:</b>	CCC=C(C)C(O)CC
<b>Mol. weight [g/mol]:</b>	128.21
<b>CAS:</b>	81280-12-8

## Physical Properties

Property code	Value	Unit	Source
gf	-51.11	kJ/mol	Joback Method
hf	-258.53	kJ/mol	Joback Method
hfus	15.93	kJ/mol	Joback Method
hvap	49.73	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.114		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
tb	478.22	K	Joback Method
tc	651.29	K	Joback Method
tf	206.70	K	Joback Method
vc	0.477	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.37	J/mol×K	478.22	Joback Method
cpg	285.03	J/mol×K	507.07	Joback Method
cpg	296.16	J/mol×K	535.91	Joback Method
cpg	306.79	J/mol×K	564.76	Joback Method
cpg	316.94	J/mol×K	593.60	Joback Method
cpg	326.63	J/mol×K	622.45	Joback Method
cpg	335.88	J/mol×K	651.29	Joback Method

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39010e+01
Coeff. B	-3.79641e+03
Coeff. C	-6.68480e+01
Temperature range (K), min.	345.72
Temperature range (K), max.	508.83

## Sources

<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=C81280128&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C81280128&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</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>

## 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>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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

**vc:** Critical Volume

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