

# Bicyclo[4.1.0]heptan-3-ol, 4,7,7-trimethyl-, (1 «alpha»,3 «beta»,4 «alpha»,6 «alpha»)-

Other names:	4,7,7-Trimethylbicyclo[4.1.0]heptan-3-ol, (1 «alpha»,3 «beta»,4 «alpha»,6 «alpha»)- (1 «alpha»,3 «beta»,4 «alpha»,6 «alpha»)-4,7,7-trimethylbicyclo[4.1.0]heptan-3-ol
Inchi:	InChI=1S/C10H18O/c1-6-4-7-8(5-9(6)11)10(7,2)3/h6-9,11H,4-5H2,1-3H3/t6-,7-,8+,9-/m1
InchiKey:	WHXOMZVLSNHION-LURQLKTLA-N
Formula:	C10H18O
SMILES:	CC1CC2C(CC1O)C2(C)C
Mol. weight [g/mol]:	154.25
CAS:	54750-09-3

## Physical Properties

Property code	Value	Unit	Source
chl	-6195.50 ± 1.20	kJ/mol	NIST Webbook
gf	-22.72	kJ/mol	Joback Method
hf	-234.10 ± 4.10	kJ/mol	NIST Webbook
hfl	-312.10 ± 1.30	kJ/mol	NIST Webbook
hfus	16.83	kJ/mol	Joback Method
hvap	78.00	kJ/mol	NIST Webbook
log10ws	-2.21		Crippen Method
logp	2.049		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	2906.11	kPa	Joback Method
tb	524.36	K	Joback Method
tc	717.42	K	Joback Method
tf	306.82	K	Joback Method
vc	0.515	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.48	J/molxK	524.36	Joback Method
cpg	372.00	J/molxK	556.54	Joback Method
cpg	387.53	J/molxK	588.71	Joback Method
cpg	402.17	J/molxK	620.89	Joback Method
cpg	416.03	J/molxK	653.07	Joback Method

cpg	429.20	J/mol×K	685.24	Joback Method
cpg	441.78	J/mol×K	717.42	Joback Method

## 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=C54750093&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C54750093&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>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<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>hfl:</b>	Liquid phase 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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