

# Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl, acetate

Inchi:	InChI=1S/C12H20O2/c1-8(13)14-10-7-9-5-6-12(10,4)11(9,2)3/h9-10H,5-7H2,1-4H3
InchiKey:	KGEKLUUHTZCSIP-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	CC(=O)OC1CC2CCC1(C)C2(C)C
Mol. weight [g/mol]:	196.29

## Physical Properties

Property code	Value	Unit	Source
gf	-100.76	kJ/mol	Joback Method
hf	-406.57	kJ/mol	Joback Method
hfus	13.34	kJ/mol	Joback Method
hvap	48.54	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.764		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinsol	1595.00		NIST Webbook
tb	559.14	K	Joback Method
tc	774.82	K	Joback Method
tf	368.84	K	Joback Method
vc	0.631	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.90	J/mol×K	559.14	Joback Method
cpg	456.54	J/mol×K	595.09	Joback Method
cpg	474.00	J/mol×K	631.03	Joback Method
cpg	490.47	J/mol×K	666.98	Joback Method
cpg	506.18	J/mol×K	702.93	Joback Method
cpg	521.34	J/mol×K	738.88	Joback Method
cpg	536.18	J/mol×K	774.82	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R591230&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R591230&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>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<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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