

# cis-2-acetoxy-1,8-cineole

<b>Inchi:</b>	InChI=1S/C12H20O3/c1-8(13)14-10-7-9-5-6-12(10,4)15-11(9,2)3/h9-10H,5-7H2,1-4H3/t9
<b>InchiKey:</b>	XRKZFWIYZDOQO-NHCYSSNCSA-N
<b>Formula:</b>	C12H20O3
<b>SMILES:</b>	CC(=O)OC1CC2CCC1(C)OC2(C)C
<b>Mol. weight [g/mol]:</b>	212.29

## Physical Properties

Property code	Value	Unit	Source
gf	-198.98	kJ/mol	Joback Method
hf	-544.73	kJ/mol	Joback Method
hfus	19.22	kJ/mol	Joback Method
hvap	53.22	kJ/mol	Joback Method
log10ws	-2.68		Crippen Method
logp	2.286		Crippen Method
mcvol	171.530	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
ripol	1797.00		NIST Webbook
ripol	1797.00		NIST Webbook
tb	590.36	K	Joback Method
tc	811.40	K	Joback Method
tf	391.89	K	Joback Method
vc	0.644	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.00	J/mol×K	590.36	Joback Method
cpg	490.68	J/mol×K	627.20	Joback Method
cpg	508.27	J/mol×K	664.04	Joback Method
cpg	525.00	J/mol×K	700.88	Joback Method
cpg	541.09	J/mol×K	737.72	Joback Method
cpg	556.75	J/mol×K	774.56	Joback Method
cpg	572.21	J/mol×K	811.40	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=R301285&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R301285&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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>ripol:</b>	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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