

# Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate, (1 «alpha»,2 «alpha»,5 «beta»)-

Other names:

Menthol, acetate, neo-  
Menthol, acetate, trans-1,3,trans-1,4-  
Neomenthol acetate  
Neomenthyl acetate

**Inchi:** InChI=1S/C12H22O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h8-9,11-12H,5-7H2,1-4H3/t9

**InchiKey:** XHXUANMFYXWVNG-USWWRNFRSA-N

**Formula:** C12H22O2

**SMILES:** CC(=O)OC1CC(C)CCC1C(C)C

**Mol. weight [g/mol]:** 198.30

**CAS:** 2230-87-7

## Physical Properties

Property code	Value	Unit	Source
gf	-177.17	kJ/mol	Joback Method
hf	-527.45	kJ/mol	Joback Method
hfus	20.08	kJ/mol	Joback Method
hvap	50.89	kJ/mol	Joback Method
log10ws	-2.99		Crippen Method
logp	3.010		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2110.00	kPa	Joback Method
rinpol	1274.00		NIST Webbook
rinpol	1262.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1274.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1569.00		NIST Webbook
tb	560.02	K	Joback Method
tc	763.29	K	Joback Method
tf	281.06	K	Joback Method
vc	0.656	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.30	J/molxK	560.02	Joback Method
cpg	476.71	J/molxK	593.90	Joback Method
cpg	496.13	J/molxK	627.78	Joback Method
cpg	514.55	J/molxK	661.66	Joback Method
cpg	531.98	J/molxK	695.54	Joback Method
cpg	548.42	J/molxK	729.41	Joback Method
cpg	563.88	J/molxK	763.29	Joback Method
dvisc	0.0032505	Paxs	281.06	Joback Method
dvisc	0.0015430	Paxs	327.55	Joback Method
dvisc	0.0008815	Paxs	374.05	Joback Method
dvisc	0.0005700	Paxs	420.54	Joback Method
dvisc	0.0004019	Paxs	467.03	Joback Method
dvisc	0.0003020	Paxs	513.53	Joback Method
dvisc	0.0002379	Paxs	560.02	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=C2230877&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2230877&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>rinpol:</b>	Non-polar retention indices
<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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