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	1275.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1262.00		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/mol×K	560.02	Joback Method
cpg	476.71	J/mol×K	593.90	Joback Method
cpg	496.13	J/mol×K	627.78	Joback Method
cpg	514.55	J/mol×K	661.66	Joback Method
cpg	531.98	J/mol×K	695.54	Joback Method
cpg	548.42	J/mol×K	729.41	Joback Method
cpg	563.88	J/mol×K	763.29	Joback Method
dvisc	0.0032505	Pa×s	281.06	Joback Method
dvisc	0.0015430	Pa×s	327.55	Joback Method
dvisc	0.0008815	Pa×s	374.05	Joback Method
dvisc	0.0005700	Pa×s	420.54	Joback Method
dvisc	0.0004019	Pa×s	467.03	Joback Method
dvisc	0.0003020	Pa×s	513.53	Joback Method
dvisc	0.0002379	Pa×s	560.02	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2230877&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume