Menthyl acetate

Other names:	(+/-)-Menthol acetate
	2-Isopropyl-5-methylcyclohexyl acetate, (1«alpha»,2«beta»,5«alpha»)-
	2-Isopropyl-5-methylcyclohexyl acetate, (1Â«alphaÂ»,2Â«betaÂ»,5Â«alphaÂ»)-
	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate, (1R,2S,5R)-rel-
	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate, (1«alpha»,2«beta»,5«alpha»)-
	Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate, (1Â«alphaÂ»,2Â«betaÂ»,5Â«alphaÂ»)-
	Menthol, acetate, cis-1,3,trans-1,4-
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-ADEWGFFLSA-N
Formula:	C12H22O2
SMILES:	CC(=O)OC1CC(C)CCC1C(C)C
Mol. weight [g/mol]:	198.30
CAS:	89-48-5

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	1299.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1276.80		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1287.00		NIST Webbook

rinpol	1286.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1277.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1279.20		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1280.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1276.80		NIST Webbook
rinpol	1288.20		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1297.00		NIST Webbook
rinpol	1300.00		NIST Webbook
rinpol	1294.70		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1302.00		NIST Webbook
rinpol	1278.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1294.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1585.00		NIST Webbook
ripol	1556.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1600.00		NIST Webbook
ripol	1560.00		NIST Webbook
ripol	1539.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1551.00		NIST Webbook
ripol	1535.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1540.00		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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41268e+01
Coeff. B	-4.16767e+03
Coeff. C	-8.04700e+01
Temperature range (K), min.	381.62
Temperature range (K), max.	553.25

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C89485&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
pvap:	Vapor 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