Dihydrocarvyl acetate

Other names:	Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, acetate, (1«alpha»,2«beta»,5«alpha»)- p-Menth-8-en-2-ol, acetate Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, acetate, (1R,2R,5R)-rel- Dihydrocarveol acetate Dihydrocarveyl acetate p-Menth-8-en-2-yl acetate 2-Methyl-5-(1-methylethenyl)cyclohexyl acetate, (1«alpha»,2«beta»,5«alpha»)- 5-Isopropenyl-2-methylcyclohexyl acetate, (1«alpha»,2«beta»,5«alpha»)- p-Mentha-8-en-2-ol, acetate Tuberyl acetate 8-p-Menthen-2-yl acetate Carhydrine Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, 1-acetate, (1R,2R,5R)-rel- Dihydrocarveol acetate (Isomer 2) 2-Methyl-5-(1-methylethenyl)-cyclohexyl acetate (1«alpha»,2«beta»,5«alpha»)-2-methyl-5-(1-methylvinyl)cyclohexyl acetate
Inchi:	InChI=1S/C12H20O2/c1-8(2)11-6-5-9(3)12(7-11)14-10(4)13/h9,11-12H,1,5-7H2,2-4H3
InchiKey:	TUSIZTVSUSBSQI-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	C=C(C)C1CCC(C)C(OC(C)=O)C1
Mol. weight [g/mol]:	196.29
CAS:	20777-49-5

Physical Properties

Property code	Value	Unit	Source
gf	-95.44	kJ/mol	Joback Method
hf	-406.53	kJ/mol	Joback Method
hfus	21.01	kJ/mol	Joback Method
hvap	50.68	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.930		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1304.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1282.00		NIST Webbook

rinpol	1292.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1319.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1348.00		NIST Webbook
rinpol	1289.00		NIST Webbook
rinpol	1308.00		NIST Webbook
rinpol	1344.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1306.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1323.00		NIST Webbook
rinpol	1305.00		NIST Webbook
rinpol	1307.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1657.00		NIST Webbook
ripol	1699.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1670.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1699.00		NIST Webbook
tb	506.20	K	NIST Webbook
tc	763.76	K	Joback Method
tf	280.34	K	Joback Method
vc	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.53	J/mol×K	557.02	Joback Method
cpg	455.28	J/mol×K	591.48	Joback Method
cpg	474.03	J/mol×K	625.93	Joback Method
cpg	491.78	J/mol×K	660.39	Joback Method
cpg	508.54	J/mol×K	694.85	Joback Method
cpg	524.33	J/mol×K	729.31	Joback Method
cpg	539.15	J/mol×K	763.76	Joback Method

Sources

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=C20777495&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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