

p-Menth-8-en-3-ol, acetate

Other names:	2-Isopropenyl-5-methylcyclohexyl acetate Cyclohexanol, 5-methyl-2-(1-methylethenyl)-, acetate 1-Methyl-4-isopropenylcyclohexan-3-yl acetate Isopulegyl acetate
Inchi:	InChI=1S/C12H20O2/c1-8(2)11-6-5-9(3)7-12(11)14-10(4)13/h9,11-12H,1,5-7H2,2-4H3
InchiKey:	HLHIVJRLSDUCI-UHFFFAOYSA-N
Formula:	C12H20O2
SMILES:	C=C(C)C1CCC(C)CC1OC(C)=O
Mol. weight [g/mol]:	196.29
CAS:	89-49-6

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	1268.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1281.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1267.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1260.00		NIST Webbook
rinpol	1271.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1259.00		NIST Webbook
rinpol	1258.00		NIST Webbook
rinpol	1258.00		NIST Webbook

ripol	1608.00		NIST Webbook
ripol	1585.00		NIST Webbook
ripol	1608.00		NIST Webbook
ripol	1581.00		NIST Webbook
ripol	1576.00		NIST Webbook
ripol	1585.00		NIST Webbook
tb	557.02	K	Joback Method
tc	763.76	K	Joback Method
tf	280.34	K	Joback Method
vc	0.644	m ³ /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

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=C89496&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
r_{ipol}:	Polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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