Menthenyl acetate

Inchi: InChI=1S/C12H20O2/c1-9(2)11-5-7-12(4,8-6-11)14-10(3)13/h5,7,9,11H,6,8H2,1-4H3/t11
InchiKey: LPDOWSQWTWVDLO-RYUDHWBXSA-N
Formula: C12H20O2
SMILES: CC(=O)OC1(C)C=CC(C(C)C)CC1
Mol. weight [g/mol]: 196.29

Physical Properties

Property code	Value	Unit	Source
gf	-144.99	kJ/mol	Joback Method
hf	-434.09	kJ/mol	Joback Method
hfus	13.93	kJ/mol	Joback Method
hvap	50.34	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.930		Crippen Method
mcvol	172.220	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	1364.00		NIST Webbook
rinpol	1364.00		NIST Webbook
tb	564.09	K	Joback Method
tc	777.47	K	Joback Method
tf	309.96	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.92	J/mol×K	564.09	Joback Method
cpg	453.66	J/mol×K	599.65	Joback Method
cpg	471.35	J/mol×K	635.22	Joback Method
cpg	488.08	J/mol×K	670.78	Joback Method
cpg	503.94	J/mol×K	706.35	Joback Method
cpg	519.03	J/mol×K	741.91	Joback Method
cpg	533.45	J/mol×K	777.47	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R204005&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume