(E)-Ocimenyl acetate

Inchi: InChI=1S/C12H18O2/c1-6-10(4)8-12(7-9(2)3)14-11(5)13/h6-8,12H,1H2,2-5H3/b10-8+
InchiKey: ZOOSZTPUIIHGKF-CSKARUKUSA-N
Formula: C12H18O2
SMILES: C=CC(C)=CC(C=C(C)C)OC(C)=O
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
gf	44.98	kJ/mol	Joback Method
hf	-200.80	kJ/mol	Joback Method
hfus	22.60	kJ/mol	Joback Method
hvap	50.48	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.017		Crippen Method
mcvol	174.480	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
ripol	1661.00		NIST Webbook
tb	554.57	K	Joback Method
tc	751.89	K	Joback Method
tf	242.32	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.13	J/mol×K	554.57	Joback Method
cpg	422.29	J/mol×K	587.46	Joback Method
cpg	436.63	J/mol×K	620.34	Joback Method
cpg	450.20	J/mol×K	653.23	Joback Method
cpg	463.04	J/mol×K	686.12	Joback Method
cpg	475.19	J/mol×K	719.01	Joback Method
cpg	486.68	J/mol×K	751.89	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=R234338&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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