8-acetoxylinalool

Inchi: InChI=1S/C12H20O3/c1-5-12(4,14)8-6-7-10(2)9-15-11(3)13/h5,7,14H,1,6,8-9H2,2-4H3/b
InchiKey: BOJXRPGLMTUOEQ-JXMROGBWSA-N
Formula: C12H20O3
SMILES: C=CC(C)(O)CCC=C(C)COC(C)=O
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
gf	-158.23	kJ/mol	Joback Method
hf	-463.93	kJ/mol	Joback Method
hfus	23.91	kJ/mol	Joback Method
hvap	66.21	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.213		Crippen Method
mcvol	184.650	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
ripol	2362.00		NIST Webbook
tb	639.92	K	Joback Method
tc	823.40	K	Joback Method
tf	339.60	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	489.33	J/mol×K	639.92	Joback Method
cpg	502.43	J/mol×K	670.50	Joback Method
cpg	514.84	J/mol×K	701.08	Joback Method
cpg	526.57	J/mol×K	731.66	Joback Method
cpg	537.68	J/mol×K	762.24	Joback Method
cpg	548.20	J/mol×K	792.82	Joback Method
cpg	558.16	J/mol×K	823.40	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=R340344&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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