linalool oxide acetate (pyranoid)

Inchi: InChI=1S/C12H20O3/c1-6-12(5)8-7-10(14-9(2)13)11(3,4)15-12/h6,10H,1,7-8H2,2-5H3/t1
InchiKey: IRWLDXUJBJPFNV-ZYHUDNBSSA-N
Formula: C12H20O3
SMILES: C=CC1(C)CCC(OC(C)=O)C(C)(C)O1
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
gf	-183.99	kJ/mol	Joback Method
hf	-498.26	kJ/mol	Joback Method
hfus	17.70	kJ/mol	Joback Method
hvap	52.81	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.452		Crippen Method
mcvol	178.090	ml/mol	McGowan Method
pc	2351.92	kPa	Joback Method
rinpol	1286.00		NIST Webbook
rinpol	1286.00		NIST Webbook
tb	584.57	K	Joback Method
tc	802.13	K	Joback Method
tf	368.67	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	466.51	J/mol×K	584.57	Joback Method
cpg	484.78	J/mol×K	620.83	Joback Method
cpg	502.05	J/mol×K	657.09	Joback Method
cpg	518.51	J/mol×K	693.35	Joback Method
cpg	534.33	J/mol×K	729.61	Joback Method
cpg	549.69	J/mol×K	765.87	Joback Method
cpg	564.77	J/mol×K	802.13	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=C56752502&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

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