trans-Linalool oxide acetate (pyranoid)

Other names:	trans-Linalool oxide (pyranoid), acetate trans-Linalool oxide acetate (E)-linalool oxide acetate pyr 2H-Pyran-3-ol, 6-ethenyltetrahydro-2,2,6-trimethyl-, 3-acetate, (3R,6S)-rel- linalool Oxide qacetate linalool oxide acetate
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
InchiKey:	IRWLDXUJBJPFNV-UHFFFAOYSA-N
Formula:	C12H20O3
SMILES:	C=CC1(C)CCC(OC(C)=O)C(C)(C)O1
Mol. weight [g/mol]:	212.29
CAS:	56752-50-2

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	1292.00		NIST Webbook
rinpol	1282.70		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1292.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1282.70		NIST Webbook
ripol	1619.00		NIST Webbook
ripol	1619.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56752502&Units=SI

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

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

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