

(Z)-Linalool oxide acetate pyranoid

Other names:	cis-Acetoxylinallol oxide
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-CMPLNLGQSA-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
ripol	1610.00		NIST Webbook
ripol	1612.00		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:	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=R315130&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	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

Latest version available from:

<https://www.chemeo.com/cid/29-005-4/Z-Linalool-oxide-acetate-pyranoid.pdf>

Generated by Cheméo on 2025-12-21 23:26:31.920555835 +0000 UTC m=+6107789.450596490.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.