

Linalool oxide (pyranoid), trans, «beta»-D-glucopyranoside, TFA

Inchi:	InChI=1S/C24H24F12O11/c1-5-20(4)7-6-10(19(2,3)47-20)43-14-13(46-18(40)24(34,35)3
InchiKey:	LPTRVPJKVCENCW-DPGMLDRLSA-N
Formula:	C24H24F12O11
SMILES:	C=CC1(C)CCC(OC2OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C2O
Mol. weight [g/mol]:	716.42

Physical Properties

Property code	Value	Unit	Source
gf	-3308.58	kJ/mol	Joback Method
hf	-4159.92	kJ/mol	Joback Method
hfus	69.73	kJ/mol	Joback Method
hvap	98.12	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	4.158		Crippen Method
mcvol	391.610	ml/mol	McGowan Method
pc	819.60	kPa	Joback Method
rinsol	1814.00		NIST Webbook
tb	1116.56	K	Joback Method
tc	1391.56	K	Joback Method
tf	776.37	K	Joback Method
vc	1.544	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1499.95	J/mol×K	1116.56	Joback Method
cpg	1527.25	J/mol×K	1162.39	Joback Method
cpg	1555.56	J/mol×K	1208.23	Joback Method
cpg	1585.33	J/mol×K	1254.06	Joback Method
cpg	1617.00	J/mol×K	1299.89	Joback Method
cpg	1651.02	J/mol×K	1345.72	Joback Method
cpg	1687.81	J/mol×K	1391.56	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R184842&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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