(Z)-Linalol furanoxide «beta»-D-glucopyranoside, TFA

Other names: Linalool oxide (furanoid), cis, «beta»-D-glucopyranoside, TFA

Inchi: InChI=1S/C24H24F12O11/c1-5-20(4)7-6-10(46-20)19(2,3)47-14-13(45-18(40)24(34,35)3

InchiKey: WJLOKMGYFMOJBB-DPGMLDRLSA-N

Formula: C24H24F12O11

SMILES: C=CC1(C)CCC(C(C)(C)OC2OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F

Mol. weight [g/mol]: 716.42

Physical Properties

Property code	Value	Unit	Source
gf	-3280.44	kJ/mol	Joback Method
hf	-4157.41	kJ/mol	Joback Method
hfus	69.65	kJ/mol	Joback Method
hvap	98.11	kJ/mol	Joback Method
log10ws	-6.26		Crippen Method
logp	4.158		Crippen Method
mcvol	391.610	ml/mol	McGowan Method
pc	811.22	kPa	Joback Method
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1784.00		NIST Webbook
tb	1113.49	K	Joback Method
tc	1388.78	K	Joback Method
tf	762.65	K	Joback Method
vc	1.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1467.29	J/mol×K	1113.49	Joback Method
cpg	1485.73	J/mol×K	1159.37	Joback Method
cpg	1503.80	J/mol×K	1205.25	Joback Method
cpg	1521.84	J/mol×K	1251.14	Joback Method
cpg	1540.18	J/mol×K	1297.02	Joback Method
cpg	1559.19	J/mol×K	1342.90	Joback Method

cpg	1579.19	J/mol×K	1388.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R184802&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume