furanlinalyloxide 6-O-(«beta»-D-apiofuranosyl)-«beta»-D-glucopyranc TFA

InChI: InChI=1S/C33H30F18O17/c1-5-26(4)7-6-12(66-26)25(2,3)67-17-15(64-22(55)31(43,44)4

InchiKey: FGBDKAZTUKSWQV-GGZOKKFMSA-N

Formula: C33H30F18O17

SMILES: C=CC1(C)CCC(C(C)(C)OC2OC(COC3OCC(COC(=O)C(F)(F)F)(OC(=O)C(F)(F)F)C3OC

Mol. weight [g/mol]: 1040.55

Physical Properties

Property code	Value	Unit	Source
gf	-5011.16	kJ/mol	Joback Method
hf	-6256.11	kJ/mol	Joback Method
hfus	101.13	kJ/mol	Joback Method
hvap	134.37	kJ/mol	Joback Method
log10ws	-7.98		Crippen Method
logp	4.849		Crippen Method
mcvol	544.800	ml/mol	McGowan Method
pc	520.78	kPa	Joback Method
rinpol	2167.00		NIST Webbook
tb	1516.70	K	Joback Method
tc	2298.89	K	Joback Method
tf	1091.90	K	Joback Method
vc	2.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2387.33	J/mol×K	1516.70	Joback Method
cpg	2554.90	J/mol×K	1647.07	Joback Method
cpg	2774.70	J/mol×K	1777.43	Joback Method
cpg	3059.65	J/mol×K	1907.80	Joback Method
cpg	3422.67	J/mol×K	2038.16	Joback Method
cpg	3876.66	J/mol×K	2168.53	Joback Method
cpg	4434.54	J/mol×K	2298.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R438689&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