3,6-Epoxy-7-megastigmen-5,9-diol «beta»-D-glucopyranoside, TFA

Inchi: InChI=1S/C29H27F15O13/c1-10(5-6-24-22(2,3)7-11(56-24)8-23(24,4)57-21(49)29(42,43

InchiKey: GTJANXDGUFHEMQ-JHHWZQCUSA-N

Formula: C29H27F15O13

SMILES: CC(C=CC12OC(CC1(C)C)CC2(C)OC(=O)C(F)(F)F)OC1OC(COC(=O)C(F)(F)F)C(OC(=C

Mol. weight [g/mol]: 868.49

Physical Properties

Property code	Value	Unit	Source
gf	-4012.59	kJ/mol	Joback Method
hf	-5018.13	kJ/mol	Joback Method
hfus	81.29	kJ/mol	Joback Method
hvap	113.31	kJ/mol	Joback Method
log10ws	-7.65		Crippen Method
logp	5.022		Crippen Method
mcvol	463.950	ml/mol	McGowan Method
pc	657.46	kPa	Joback Method
rinpol	2340.00		NIST Webbook
tb	1307.31	K	Joback Method
tc	1734.51	K	Joback Method
tf	939.63	K	Joback Method
vc	1.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2018.13	J/mol×K	1307.31	Joback Method
cpg	2124.34	J/mol×K	1378.51	Joback Method
cpg	2249.07	J/mol×K	1449.71	Joback Method
cpg	2395.21	J/mol×K	1520.91	Joback Method
cpg	2565.65	J/mol×K	1592.11	Joback Method
cpg	2763.28	J/mol×K	1663.31	Joback Method
cpg	2991.01	J/mol×K	1734.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R330406&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