(6S,9R)-Vomifolyl 9-O-«beta»-D-glucopyranoside, TFA

Inchi: InChI=1S/C29H25F15O13/c1-10-7-12(45)8-23(3,4)24(10,57-22(50)29(42,43)44)6-5-11(2

InchiKey: MIHGVFQWWLBUMI-HNVNEJNSSA-N

Formula: C29H25F15O13

SMILES: CC1=CC(=O)CC(C)(C)C1(C=CC(C)OC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC

Mol. weight [g/mol]: 866.48

Physical Properties

Property code	Value	Unit	Source
gf	-4100.48	kJ/mol	Joback Method
hf	-5057.54	kJ/mol	Joback Method
hfus	76.55	kJ/mol	Joback Method
hvap	115.89	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	4.990		Crippen Method
mcvol	466.210	ml/mol	McGowan Method
pc	648.45	kPa	Joback Method
rinpol	2317.00		NIST Webbook
tb	1358.55	K	Joback Method
tc	1820.86	K	Joback Method
tf	949.92	K	Joback Method
vc	1.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1886.41	J/mol×K	1358.55	Joback Method
cpg	1948.01	J/mol×K	1435.60	Joback Method
cpg	2018.74	J/mol×K	1512.65	Joback Method
cpg	2100.76	J/mol×K	1589.71	Joback Method
cpg	2196.21	J/mol×K	1666.76	Joback Method
cpg	2307.24	J/mol×K	1743.81	Joback Method
cpg	2435.99	J/mol×K	1820.86	Joback Method

Sources

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=R330411&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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