Vomifoliol, «beta»-D-glucopyranoside, TFA

Inchi: InChI=1S/C28H23F15O13/c1-10(4-6-23(56-21(49)28(41,42)43)7-5-11(44)8-22(23,2)3)51
InchiKey: IRFPMKAVAOLFLX-IXQDIEQASA-N
Formula: C28H23F15O13
SMILES: CC(C=CC1(OC(=O)C(F)(F)F)C=CC(=O)CC1(C)C)OC1OC(COC(=O)C(F)(F)F)C(OC(=O)
Mol. weight [g/mol]: 852.45

Physical Properties

Property code	Value	Unit	Source
gf	-4099.27	kJ/mol	Joback Method
hf	-5025.43	kJ/mol	Joback Method
hfus	74.35	kJ/mol	Joback Method
hvap	113.01	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	4.600		Crippen Method
mcvol	452.120	ml/mol	McGowan Method
pc	686.73	kPa	Joback Method
rinpol	2319.00		NIST Webbook
tb	1330.69	K	Joback Method
tc	1759.15	K	Joback Method
tf	926.13	K	Joback Method
vc	1.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1813.56	J/mol×K	1330.69	Joback Method
cpg	1868.02	J/mol×K	1402.10	Joback Method
cpg	1929.95	J/mol×K	1473.51	Joback Method
cpg	2001.10	J/mol×K	1544.92	Joback Method
cpg	2083.19	J/mol×K	1616.33	Joback Method
cpg	2177.97	J/mol×K	1687.74	Joback Method
cpg	2287.18	J/mol×K	1759.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R184906&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume