Scopoletin «beta»-D-glucopyranoside, TFA

Inchi: InChI=1S/C24H14F12O13/c1-42-9-4-7-2-3-12(37)44-8(7)5-10(9)45-16-15(49-20(41)24(3
InchiKey: LCASGYIODNQINV-YMILTQATSA-N
Formula: C24H14F12O13
SMILES: COc1cc2ccc(=O)oc2cc1OC1OC(COC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F
Mol. weight [g/mol]: 738.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.25		Crippen Method
logp	3.433		Crippen Method
mcvol	375.290	ml/mol	McGowan Method
rinpol	2510.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R330500&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices