Scopoletin, O-heptafluorobutyryl-

Inchi: InChI=1S/C14H7F7O5/c1-24-8-4-6-2-3-10(22)25-7(6)5-9(8)26-11(23)12(15,16)13(17,18)14(19,20)21/h2-5H,1H3

InchiKey: CMDJHAUPXYOUNX-UHFFFAOYSA-N

Formula: C14H7F7O5

SMILES: COc1cc2ccc(=O)oc2cc1OC(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 388.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.99		Crippen Method
logp	3.540		Crippen Method
mcvol	202.340	ml/mol	McGowan Method
rinpol	1867.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374302&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices