Scopoletin, O-pentafluoropropionyl-

Inchi: InChI=1S/C13H7F5O5/c1-21-8-4-6-2-3-10(19)22-7(6)5-9(8)23-11(20)12(14,15)13(16,17)18/h2-5H,1H3
InchiKey: SZAQXVKWHIHWAK-UHFFFAOYSA-N
Formula: C13H7F5O5
SMILES: COc1cc2ccc(=O)oc2cc1OC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 338.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.26		Crippen Method
logp	2.905		Crippen Method
mcvol	184.710	ml/mol	McGowan Method
rinpol	1825.00		NIST Webbook
rinpol	1825.00		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=U374303&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

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