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)
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: 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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374303&Units=SI

Legend

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

Latest version available from:
https://www.chemeo.com/cid/49-347-3/Scopoletin-O-pentafluoropropionyl.pdf
Generated by Cheméo on 2024-04-28 23:05:05.011033125 +0000 UTC m=+16634753.931610440.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.