Scopoletin, O-trifluoroacetyl-

Inchi: InChI=1S/C12H7F3O5/c1-18-8-4-6-2-3-10(16)19-7(6)5-9(8)20-11(17)12(13,14)15/h2-5H,
InchiKey: XHIACJDQFMGLNV-UHFFFAOYSA-N
Formula: C12H7F3O5
SMILES: COc1cc2ccc(=O)oc2cc1OC(=O)C(F)(F)F
Mol. weight [g/mol]: 288.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.53		Crippen Method
logp	2.269		Crippen Method
mcvol	167.080	ml/mol	McGowan Method
rinpol	1810.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374304&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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