

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)
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
rinsol	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/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/10-019-9/Scopoletin-O-heptafluorobutyryl.pdf>

Generated by Cheméo on 2024-04-18 07:14:42.865149107 +0000 UTC m=+15713731.785726422.

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