

Indoleacetic acid, methyl, 1-PFP

Inchi: InChI=1S/C14H10F5NO3/c1-23-11(21)6-8-7-20(10-5-3-2-4-9(8)10)12(22)13(15,16)14(17)
InchiKey: HVCYLVDDRIHNLM-UHFFFAOYSA-N
Formula: C14H10F5NO3
SMILES: COC(=O)Cc1cn(C(=O)C(F)(F)C(F)(F)F)c2ccccc12
Mol. weight [g/mol]: 335.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Crippen Method
logp	3.195		Crippen Method
mcvol	197.040	ml/mol	McGowan Method
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R580057&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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