

8-Methyl-8-azabicyclo[3.2.1]octan-3-yl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C15H14F5NO2/c1-21-6-2-3-7(21)5-8(4-6)23-15(22)9-10(16)12(18)14(20)13(19)
InchiKey: VJZOOQCJGZKBPE-UHFFFAOYSA-N
Formula: C15H14F5NO2
SMILES: CN1C2CCC1CC(OC(=O)c1c(F)c(F)c(F)c(F)c1F)C2
Mol. weight [g/mol]: 335.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.00		Crippen Method
logp	3.164		Crippen Method
mcvol	203.000	ml/mol	McGowan Method
rinpol	1784.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U373606&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

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