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/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=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