

Isonipecotic acid, N-pentafluorobenzoyl-, decyl ester

Inchi: InChI=1S/C23H30F5NO3/c1-2-3-4-5-6-7-8-9-14-32-23(31)15-10-12-29(13-11-15)22(30)1
InchiKey: BVURMDDPNWXNTH-UHFFFAOYSA-N
Formula: C23H30F5NO3
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)c2c(F)c(F)c(F)c2F)CC1
Mol. weight [g/mol]: 463.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.65		Crippen Method
logp	5.918		Crippen Method
mcvol	328.150	ml/mol	McGowan Method
rinpol	2797.00		NIST Webbook
rinpol	2797.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361230&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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

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