

Isonipecotic acid, N-pentafluorobenzoyl-, undecyl ester

Inchi: InChI=1S/C24H32F5NO3/c1-2-3-4-5-6-7-8-9-10-15-33-24(32)16-11-13-30(14-12-16)23(3)
InchiKey: FRXUAROKIUFIDY-UHFFFAOYSA-N
Formula: C24H32F5NO3
SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2c(F)c(F)c(F)c(F)c2F)CC1
Mol. weight [g/mol]: 477.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.07		Crippen Method
logp	6.308		Crippen Method
mcvol	342.240	ml/mol	McGowan Method
rinpol	2907.00		NIST Webbook
rinpol	2907.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361231&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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