

Isonipecotic acid, N-(3-fluoro-4-trifluoromethylbenzoyl)-, pentadecyl ester

InChI: InChI=1S/C29H43F4NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-21-37-28(36)23-17-19-34(2)
InChIKey: PUUGJDNLBVRMFJ-UHFFFAOYSA-N

Formula: C29H43F4NO3
SMILES: CCCCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(C(F)(F)F)c(F)c2)CC1
Mol. weight [g/mol]: 529.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.52		Crippen Method
logp	8.331		Crippen Method
mcvol	410.920	ml/mol	McGowan Method
rinpole	3461.00		NIST Webbook

Sources

Crippen Method: https://www.cheméo.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=U361479&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

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