

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

InChI: InChI=1S/C25H35F4NO3/c1-2-3-4-5-6-7-8-9-10-17-33-24(32)19-13-15-30(16-14-19)23(31)18
InChIKey: GKWWYIBYNPHTPJ-UHFFFAOYSA-N

Formula: C₂₅H₃₅F₄NO₃

SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(C(F)(F)F)c(F)c2)CC1

Mol. weight [g/mol]: 473.54

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.85 | | Crippen Method |
| logp | 6.771 | | Crippen Method |
| mcvol | 354.560 | ml/mol | McGowan Method |
| rinpole | 3048.00 | | NIST Webbook |
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Sources

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

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=U361475&Units=SI>

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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