

Isonipecotic acid, N-(2-fluoro-5-trifluoromethylbenzoyl)-, dodecyl ester

InChI: InChI=1S/C26H37F4NO3/c1-2-3-4-5-6-7-8-9-10-11-18-34-25(33)20-14-16-31(17-15-20)2
InChIKey: FTOXHOGCBJNYBX-UHFFFAOYSA-N

Formula: C26H37F4NO3

SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2F)CC1

Mol. weight [g/mol]: 487.57

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -8.26 | | Crippen Method |
| logp | 7.161 | | Crippen Method |
| mcvol | 368.650 | ml/mol | McGowan Method |
| rinpole | 3101.00 | | 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=U361397&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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