

Isonipecotic acid, N-(2,5-difluorobenzoyl)-, undecyl ester

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|-----------------------------|----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C24H35F2NO3/c1-2-3-4-5-6-7-8-9-10-17-30-24(29)19-13-15-27(16-14-19)23(2 |
| InchiKey: | HOQGDGQVDFLWES-UHFFFAOYSA-N |
| Formula: | C24H35F2NO3 |
| SMILES: | CCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(F)ccc2F)CC1 |
| Mol. weight [g/mol]: | 423.54 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.07 | | Crippen Method |
| logp | 5.891 | | Crippen Method |
| mcvol | 336.930 | ml/mol | McGowan Method |
| rinpol | 3111.00 | | NIST Webbook |
| rinpol | 3111.00 | | NIST Webbook |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U361419&Units=SI |
| 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 |

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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