

Isonipecotic acid, N-(3-fluoro-6-trifluoromethylbenzoyl)-, hexyl

Inchi:
ester

InChI=1S/C20H25F4NO3/c1-2-3-4-5-12-28-19(27)14-8-10-25(11-9-14)18(26)16-13-15(2

InchiKey:

DZOWZDCAIQTWNB-UHFFFAOYSA-N

Formula:

C20H25F4NO3

SMILES:

CCCCCOC(=O)C1CCN(C(=O)c2cc(F)ccc2C(F)(F)F)CC1

Mol. weight [g/mol]:

403.41

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.75 | | Crippen Method |
| logp | 4.820 | | Crippen Method |
| mcvol | 284.110 | ml/mol | McGowan Method |
| rinpol | 2491.00 | | NIST Webbook |
| rinpol | 2491.00 | | NIST Webbook |

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361333&Units=SI>

Crippen Method:

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

Crippen Method:

https://www.chemeo.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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