

L-Proline, N-(3-fluoro-4-trifluoromethylbenzoyl)-, decyl

Inchi:
ester

InChI=1S/C23H31F4NO3/c1-2-3-4-5-6-7-8-9-15-31-22(30)20-11-10-14-28(20)21(29)17-1

InchiKey:

OTOPFAJRPJOMQM-UHFFFAOYSA-N

Formula:

C23H31F4NO3

SMILES:

CCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]:

445.49

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.36 | | Crippen Method |
| logp | 6.133 | | Crippen Method |
| mcvol | 326.380 | ml/mol | McGowan Method |
| rinpol | 2718.00 | | NIST Webbook |
| rinpol | 2718.00 | | NIST Webbook |

Sources

Crippen Method:

https://www.chemeo.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=U345969&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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<https://www.chemeo.com/cid/116-437-8/L-Proline-N-3-fluoro-4-trifluoromethylbenzoyl-decyl-ester.pdf>

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