

L-Proline, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, decyl

Inchi:
ester

InChI=1S/C23H32F3NO4/c1-3-4-5-6-7-8-9-10-14-31-23(29)18-12-11-13-27(18)22(28)16

InchiKey:

JIDWYYMJHZSEBR-UHFFFAOYSA-N

Formula:

C23H32F3NO4

SMILES:

CCCCCCCCCOC(=O)C1CCCN1C(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]:

443.50

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.04 | | Crippen Method |
| logp | 5.401 | | Crippen Method |
| mcvol | 330.480 | ml/mol | McGowan Method |
| rinpol | 2907.00 | | NIST Webbook |
| rinpol | 2907.00 | | NIST Webbook |

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U346027&Units=SI>

Crippen Method:

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

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

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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