

L-Proline, N-(3-chloro-2-fluorobenzoyl)-, decyl ester

Inchi: InChI=1S/C22H31ClFNO3/c1-2-3-4-5-6-7-8-9-16-28-22(27)19-14-11-15-25(19)21(26)17-
InchiKey: KDMZCPVBLOHTKG-UHFFFAOYSA-N
Formula: C22H31ClFNO3
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 411.94

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -6.94 | | Crippen Method |
| logp | 5.768 | | Crippen Method |
| mcvol | 319.220 | ml/mol | McGowan Method |
| rinpol | 3006.00 | | NIST Webbook |
| rinpol | 3006.00 | | NIST Webbook |

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=U345942&Units=SI>

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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