

Isonipecotic acid, N-(2-fluoro-3-chlorobenzoyl)-, octyl ester

Inchi: InChI=1S/C21H29ClFNO3/c1-2-3-4-5-6-7-15-27-21(26)16-11-13-24(14-12-16)20(25)17-9
InchiKey: AOEALGPHHISBOD-UHFFFAOYSA-N
Formula: C₂₁H₂₉ClFNO₃
SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2cccc(Cl)c2F)CC1
Mol. weight [g/mol]: 397.91

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -6.17 | | Crippen Method |
| logp | 5.235 | | Crippen Method |
| mcvol | 305.130 | ml/mol | McGowan Method |
| rinpol | 3044.00 | | NIST Webbook |
| rinpol | 3044.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361438&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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