

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

Inchi: InChI=1S/C23H33ClFNO3/c1-2-3-4-5-6-7-8-9-17-29-23(28)18-13-15-26(16-14-18)22(27)
InchiKey: ZCSZESJZQYAEIY-UHFFFAOYSA-N
Formula: C₂₃H₃₃ClFNO₃
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)c2cccc(Cl)c2F)CC1
Mol. weight [g/mol]: 425.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.01		Crippen Method
logp	6.015		Crippen Method
mcvol	333.310	ml/mol	McGowan Method
rinpole	3254.00		NIST Webbook
rinpole	3254.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361440&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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
rinpole: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/122-801-6/Isonipecotic-acid-N-2-fluoro-3-chlorobenzoyl-decyl-ester.pdf>

Generated by Cheméo on 2024-05-03 17:40:42.547392436 +0000 UTC m=+17047291.467969750.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.