

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

Inchi: InChI=1S/C19H25ClFNO3/c1-13(2)5-4-12-25-19(24)14-8-10-22(11-9-14)18(23)15-6-3-7-
InchiKey: YRCAUDJUXUTBPK-UHFFFAOYSA-N
Formula: C19H25ClFNO3
SMILES: CC(C)CCCOC(=O)C1CCN(C(=O)c2cccc(Cl)c2F)CC1
Mol. weight [g/mol]: 369.86

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.09		Crippen Method
logp	4.311		Crippen Method
mcvol	276.950	ml/mol	McGowan Method
rinpol	2771.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U361435&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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