

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

Inchi: InChI=1S/C20H27ClFNO3/c1-2-3-4-5-6-14-26-20(25)15-10-12-23(13-11-15)19(24)16-8-7
InchiKey: DYSUKIMLQYDGOR-UHFFFAOYSA-N
Formula: C20H27ClFNO3
SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2cccc(Cl)c2F)CC1
Mol. weight [g/mol]: 383.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.75		Crippen Method
logp	4.845		Crippen Method
mcvol	291.040	ml/mol	McGowan Method
rinpol	2932.00		NIST Webbook
rinpol	2932.00		NIST Webbook

Sources

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=U361437&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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