

Isonipecotic acid, N-(3,4-difluorobenzoyl)-, nonyl ester

Inchi: InChI=1S/C22H31F2NO3/c1-2-3-4-5-6-7-8-15-28-22(27)17-11-13-25(14-12-17)21(26)18
InchiKey: PPPLJKKFQKHULC-UHFFFAOYSA-N
Formula: C22H31F2NO3
SMILES: CCCCCCCCCOC(=O)C1CCN(C(=O)c2ccc(F)c(F)c2)CC1
Mol. weight [g/mol]: 395.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.24		Crippen Method
logp	5.111		Crippen Method
mcvol	308.750	ml/mol	McGowan Method
rinpol	2921.00		NIST Webbook
rinpol	2921.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=U361271&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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