

Isonipecotinoylisonipecotic acid, N'-(3,4-difluorobenzoyl)-, propyl ester

Inchi: InChI=1S/C22H28F2N2O4/c1-2-13-30-22(29)16-7-11-25(12-8-16)20(27)15-5-9-26(10-6-
InchiKey: MBPRIQPDYPSUSI-UHFFFAOYSA-N
Formula: C22H28F2N2O4
SMILES: CCCOC(=O)C1CCN(C(=O)C2CCN(C(=O)c3ccc(F)c(F)c3)CC2)CC1
Mol. weight [g/mol]: 422.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.23		Crippen Method
logp	3.009		Crippen Method
mcvol	309.440	ml/mol	McGowan Method
rinpol	3482.00		NIST Webbook
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Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361281&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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