

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

Inchi: InChI=1S/C17H21F2NO3/c1-11(2)10-23-17(22)12-5-7-20(8-6-12)16(21)13-3-4-14(18)15
InchiKey: HJPMWVGAOELPG-UHFFFAOYSA-N
Formula: C17H21F2NO3
SMILES: CC(C)COC(=O)C1CCN(C(=O)c2ccc(F)c(F)c2)CC1
Mol. weight [g/mol]: 325.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	3.016		Crippen Method
mcvol	238.300	ml/mol	McGowan Method
rinsol	2353.00		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=U361264&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

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