

Isonipecotic acid, N-(2,5-difluorobenzoyl)-, isobutyl ester

Inchi: InChI=1S/C17H21F2NO3/c1-11(2)10-23-17(22)12-5-7-20(8-6-12)16(21)14-9-13(18)3-4-1
InchiKey: UTJSEEHJNIFBAC-UHFFFAOYSA-N
Formula: C17H21F2NO3
SMILES: CC(C)COC(=O)C1CCN(C(=O)c2cc(F)ccc2F)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
rinpol	2321.00		NIST Webbook
rinpol	2321.00		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=U361410&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/28-250-3/Isonipecotic-acid-N-2-5-difluorobenzoyl-isobutyl-ester.pdf>

Generated by Cheméo on 2024-04-19 18:56:46.952968744 +0000 UTC m=+15842255.873546059.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.