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

Inchi: InChI=1S/C23H33F2NO3/c1-2-3-4-5-6-7-8-9-16-29-23(28)18-12-14-26(15-13-18)22(27)2

InchiKey: ASGDUZFUJKRAMC-UHFFFAOYSA-N

Formula: C23H33F2NO3

SMILES: CCCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(F)ccc2F)CC1

Mol. weight [g/mol]: 409.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.65		Crippen Method
logp	5.501		Crippen Method
mcvol	322.840	ml/mol	McGowan Method
rinpol	3004.00		NIST Webbook
rinpol	3004.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U361418&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/40-299-6/Isonipecotic-acid-N-2-5-difluorobenzoyl-decyl-ester.pdf
Generated by Cheméo on 2024-10-12 03:20:00.213082623 +0000 UTC m=+3284062.850051874.

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