

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

Inchi:	InChI=1S/C25H37F2NO3/c1-2-3-4-5-6-7-8-9-10-11-18-31-25(30)20-14-16-28(17-15-20)2
InchiKey:	QRHOCDFWOOJNSZ-UHFFFAOYSA-N
Formula:	C25H37F2NO3
SMILES:	CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2cc(F)ccc2F)CC1
Mol. weight [g/mol]:	437.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.49		Crippen Method
logp	6.281		Crippen Method
mcvol	351.020	ml/mol	McGowan Method
rinpol	3213.00		NIST Webbook
rinpol	3213.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361420&Units=SI
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

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.cheméo.com/cid/115-069-8/Isonipecotic-acid-N-2-5-difluorobenzoyl-dodecyl-ester.pdf>

Generated by Cheméo on 2024-04-29 09:42:14.924986611 +0000 UTC m=+16672983.845563922.

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