

Isonipecotic acid, N-(3-fluorobenzoyl)-, hexyl ester

Inchi:	InChI=1S/C19H26FNO3/c1-2-3-4-5-13-24-19(23)15-9-11-21(12-10-15)18(22)16-7-6-8-17
InchiKey:	FUISDTAITLIGCD-UHFFFAOYSA-N
Formula:	C19H26FNO3
SMILES:	CCCCCOC(=O)C1CCN(C(=O)c2cccc(F)c2)CC1
Mol. weight [g/mol]:	335.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.65		Crippen Method
logp	3.801		Crippen Method
mcvol	264.710	ml/mol	McGowan Method
rinpol	2625.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U361522&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

Latest version available from:

<https://www.chemeo.com/cid/23-806-1/Isonipecotic-acid-N-3-fluorobenzoyl-hexyl-ester.pdf>

Generated by Cheméo on 2024-04-25 19:15:35.937178343 +0000 UTC m=+16361784.857755653.

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