

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

Inchi:	InChI=1S/C19H25F2NO3/c1-13(2)4-3-11-25-19(24)14-7-9-22(10-8-14)18(23)16-12-15(20)
InchiKey:	UZWDJTITRUZTGF-UHFFFAOYSA-N
Formula:	C19H25F2NO3
SMILES:	CC(C)CCCOC(=O)C1CCN(C(=O)c2cc(F)ccc2F)CC1
Mol. weight [g/mol]:	353.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	3.796		Crippen Method
mcvol	266.480	ml/mol	McGowan Method
rinpola	2536.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361413&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
rinpola:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/32-203-0/Isonipecotic-acid-N-2-5-difluorobenzoyl-isohexyl-ester.pdf>

Generated by Cheméo on 2024-04-20 16:03:10.422913884 +0000 UTC m=+15918239.343491244.

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