

Isonipectic acid, N-(2,6-difluoro-3-methylbenzoyl)-, isohexyl

Inchi:
ester

InChI=1S/C20H27F2NO3/c1-13(2)5-4-12-26-20(25)15-8-10-23(11-9-15)19(24)17-16(21)

InchiKey:

VOEZHDBRJAEXSV-UHFFFAOYSA-N

Formula:

C20H27F2NO3

SMILES:

Cc1ccc(F)c(C(=O)N2CCC(C(=O)OCCCC(C)C)CC2)c1F

Mol. weight [g/mol]:

367.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.21		Crippen Method
logp	4.105		Crippen Method
mcvol	280.570	ml/mol	McGowan Method
rinpol	2668.00		NIST Webbook
rinpol	2668.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361302&Units=SI>

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>

Legend

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

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