

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

Inchi:
ester

InChI=1S/C18H23F2NO3/c1-11(2)10-24-18(23)13-6-8-21(9-7-13)17(22)15-14(19)5-4-12

InchiKey:

ZDRIWLXBTWDQHR-UHFFFAOYSA-N

Formula:

C18H23F2NO3

SMILES:

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

Mol. weight [g/mol]:

339.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	3.325		Crippen Method
mcvol	252.390	ml/mol	McGowan Method
rinpola	2456.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361299&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
rinpola:	Non-polar retention indices

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