

Isonipecotic acid, N-(2,6-difluoro-3-methylbenzoyl)-, tridecyl

Inchi:
ester

InChI=1S/C27H41F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-20-33-27(32)22-16-18-30(19-17

InchiKey:

XZSBRRJMMVLPDI-UHFFFAOYSA-N

Formula:

C27H41F2NO3

SMILES:

CCCCCCCCCCCCOC(=O)C1CCN(C(=O)c2c(F)ccc(C)c2F)CC1

Mol. weight [g/mol]:

465.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.39		Crippen Method
logp	6.980		Crippen Method
mcvol	379.200	ml/mol	McGowan Method
rinpola	3457.00		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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=U361305&Units=SI>

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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