

Isonipecotic acid, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, hexyl

Inchi:
ester

InChI=1S/C20H26F3NO4/c1-3-4-5-6-11-28-20(26)13-7-9-24(10-8-13)19(25)14-12-15(21)

InchiKey:

NVCQEONISUVYIZ-UHFFFAOYSA-N

Formula:

C20H26F3NO4

SMILES:

CCCCCOC(=O)C1CCN(C(=O)c2cc(F)c(F)c(OC)c2F)CC1

Mol. weight [g/mol]:

401.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.43		Crippen Method
logp	4.088		Crippen Method
mcvol	288.210	ml/mol	McGowan Method
rinpola	2725.00		NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361353&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

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