

Isonipectic acid, N-(2,5-di(trifluoromethyl)benzoyl)-, isobutyl

Inchi:
ester

InChI=1S/C19H21F6NO3/c1-11(2)10-29-17(28)12-5-7-26(8-6-12)16(27)14-9-13(18(20,2

InchiKey:

SIHPJFSISJATNW-UHFFFAOYSA-N

Formula:

C19H21F6NO3

SMILES:

CC(C)COC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2C(F)(F)F)CC1

Mol. weight [g/mol]:

425.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	4.776		Crippen Method
mcvol	273.560	ml/mol	McGowan Method
rinpol	2133.00		NIST Webbook
rinpol	2133.00		NIST Webbook

Sources

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>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361202&Units=SI>

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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