

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

Inchi:
ester

InChI=1S/C18H19F6NO3/c1-2-9-28-16(27)11-5-7-25(8-6-11)15(26)13-10-12(17(19,20)2

InchiKey:

YQMRAJVBSDGETG-UHFFFAOYSA-N

Formula:

C18H19F6NO3

SMILES:

CCCOC(=O)C1CCN(C(=O)c2cc(C(F)(F)F)ccc2C(F)(F)F)CC1

Mol. weight [g/mol]:

411.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.27		Crippen Method
logp	4.530		Crippen Method
mcvol	259.470	ml/mol	McGowan Method
rinpola	2082.00		NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361201&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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