

Isonipecotic acid, N-(2,5-di(trifluoromethyl)benzoyl)-, isoheptyl ester

InChI:
InChIKey:

InChI=1S/C21H25F6NO3/c1-13(2)4-3-11-31-19(30)14-7-9-28(10-8-14)18(29)16-12-15(20)
JCQXCVAIYKDEKY-UHFFFAOYSA-N

Formula:

C₂₁H₂₅F₆NO₃

SMILES:

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

Mol. weight [g/mol]:

453.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.28		Crippen Method
logp	5.556		Crippen Method
mcvol	301.740	ml/mol	McGowan Method
rinpol	2338.00		NIST Webbook
rinpol	2338.00		NIST Webbook

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U361205&Units=SI>

Crippen Method:

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

Crippen Method:

https://www.cheméo.com/doc/models/crippen_log10ws

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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