

Isonipectic acid, N-(3-fluoro-4-trifluoromethylbenzoyl)-, heptyl

Inchi:
ester

InChI=1S/C21H27F4NO3/c1-2-3-4-5-6-13-29-20(28)15-9-11-26(12-10-15)19(27)16-7-8-1

InchiKey:

OBAlMQNAXVAXSQ-UHFFFAOYSA-N

Formula:

C₂₁H₂₇F₄NO₃

SMILES:

CCCCCCCOC(=O)C1CCN(C(=O)c2ccc(C(F)(F)F)c(F)c2)CC1

Mol. weight [g/mol]:

417.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.17		Crippen Method
logp	5.210		Crippen Method
mcvol	298.200	ml/mol	McGowan Method
rinpole	2633.00		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=U361471&Units=SI>

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpole:	Non-polar retention indices

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