

Isonipectic acid, N-(3-fluoro-5-trifluoromethylbenzoyl)-, heptyl

Inchi:
ester

InChI=1S/C21H27F4NO3/c1-2-3-4-5-6-11-29-20(28)15-7-9-26(10-8-15)19(27)16-12-17(2

InchiKey: HVLJTRAIEIBODL-UHFFFAOYSA-N

Formula: C₂₁H₂₇F₄NO₃

SMILES: CCCCCCOC(=O)C1CCN(C(=O)c2cc(F)cc(C(F)(F)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
rinpol	2539.00		NIST Webbook
rinpol	2539.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361451&Units=SI>

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>

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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