

Isonipectic acid, N-(3-fluoro-5-trifluoromethylbenzoyl)-, pentyl ester

InChI: InChI=1S/C19H23F4NO3/c1-2-3-4-9-27-18(26)13-5-7-24(8-6-13)17(25)14-10-15(19(21,22)23)/n1
InChIKey: VCSUMUZZFJMMKJ-UHFFFAOYSA-N
Formula: C19H23F4NO3
SMILES: CCCCCOC(=O)C1CCN(C(=O)c2cc(F)cc(C(F)(F)F)c2)CC1
Mol. weight [g/mol]: 389.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.33		Crippen Method
logp	4.430		Crippen Method
mcvol	270.020	ml/mol	McGowan Method
rinpol	2339.00		NIST Webbook
rinpol	2339.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361448&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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