

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

InChI: InChI=1S/C20H25F4NO3/c1-13(2)4-3-9-28-19(27)14-5-7-25(8-6-14)18(26)15-10-16(20(21)22)17
InChIKey: CYXBAMHXIXYGOC-UHFFFAOYSA-N

Formula: C20H25F4NO3
SMILES: CC(C)CCCOC(=O)C1CCN(C(=O)c2cc(F)cc(C(F)(F)F)c2)CC1
Mol. weight [g/mol]: 403.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.51		Crippen Method
logp	4.676		Crippen Method
mcvol	284.110	ml/mol	McGowan Method
rinpole	2399.00		NIST Webbook
rinpole	2399.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U361449&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
rinpole: Non-polar retention indices

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