

Isonipectic acid, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, isoheptyl ester

InChI: InChI=1S/C20H26F3NO4/c1-12(2)5-4-10-28-20(26)13-6-8-24(9-7-13)19(25)14-11-15(21)
InChIKey: LRLCKCQQUZQXHX-UHFFFAOYSA-N

Formula: C₂₀H₂₆F₃NO₄

SMILES: COc1c(F)c(F)cc(C(=O)N2CCC(C(=O)OCCCC(C)C)CC2)c1F

Mol. weight [g/mol]: 401.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.19		Crippen Method
logp	3.944		Crippen Method
mcvol	288.210	ml/mol	McGowan Method
rinpol	2690.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.cheméo.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=U361352&Units=SI>

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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