

L-Proline, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, isohexyl ester

InChI: InChI=1S/C19H24F3NO4/c1-11(2)6-5-9-27-19(25)14-7-4-8-23(14)18(24)12-10-13(20)16
InChIKey: VLEHHFXRUAJBMH-UHFFFAOYSA-N

Formula: C19H24F3NO4
SMILES: COc1c(F)c(F)cc(C(=O)N2CCCC2C(=O)OCCCC(C)C)c1F
Mol. weight [g/mol]: 387.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.12		Crippen Method
logp	3.696		Crippen Method
mcvol	274.120	ml/mol	McGowan Method
rinpol	2447.00		NIST Webbook
rinpol	2447.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346023&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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