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

Inchi: InChI=1S/C18H22F3NO4/c1-3-4-5-9-26-18(24)13-7-6-8-22(13)17(23)11-10-12(19)15(21)
InchiKey: CNYGGQKMWZGFMO-UHFFFAOYSA-N
Formula: C18H22F3NO4
SMILES: CCCCCOC(=O)C1CCCN1C(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 373.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.95		Crippen Method
logp	3.451		Crippen Method
mcvol	260.030	ml/mol	McGowan Method
rinpol	2398.00		NIST Webbook
rinpol	2398.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346022&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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