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

Inchi: InChI=1S/C17H20F3NO4/c1-3-4-8-25-17(23)12-6-5-7-21(12)16(22)10-9-11(18)14(20)15(

InchiKey: ACXYARHMRYRDNV-UHFFFAOYSA-N

Formula: C17H20F3NO4

SMILES: CCCCOC(=O)C1CCCN1C(=O)c1cc(F)c(F)c(OC)c1F

Mol. weight [g/mol]: 359.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	3.060		Crippen Method
mcvol	245.940	ml/mol	McGowan Method
rinpol	2301.00		NIST Webbook
rinpol	2301.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.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=U346021&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.