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

Inchi: InChI=1S/C16H18F3NO4/c1-3-7-24-16(22)11-5-4-6-20(11)15(21)9-8-10(17)13(19)14(23-
InchiKey: LEXKVBDQFMKFPR-UHFFFAOYSA-N
Formula: C16H18F3NO4
SMILES: CCCOC(=O)C1CCCN1C(=O)c1cc(F)c(F)c(OC)c1F
Mol. weight [g/mol]: 345.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	2.670		Crippen Method
mcvol	231.850	ml/mol	McGowan Method
rinpol	2212.00		NIST Webbook
rinpol	2212.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346020&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

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