L-Proline, N-(3-methoxybenzoyl)-, pentyl ester

Inchi: InChI=1S/C18H25NO4/c1-3-4-5-12-23-18(21)16-10-7-11-19(16)17(20)14-8-6-9-15(13-14
InchiKey: XJEONSJXRHMHIJ-UHFFFAOYSA-N
Formula: C18H25NO4
SMILES: CCCCCOC(=O)C1CCCN1C(=O)c1cccc(OC)c1
Mol. weight [g/mol]: 319.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	3.033		Crippen Method
mcvol	254.720	ml/mol	McGowan Method
rinpol	2570.00		NIST Webbook
rinpol	2570.00		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=U346170&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

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