L-Proline, N-(2-bromobenzoyl)-, pentyl ester

Inchi: InChI=1S/C17H22BrNO3/c1-2-3-6-12-22-17(21)15-10-7-11-19(15)16(20)13-8-4-5-9-14(1
InchiKey: IDPUAYZDIYOEJO-UHFFFAOYSA-N
Formula: C17H22BrNO3
SMILES: CCCCCOC(=O)C1CCCN1C(=O)c1ccccc1Br
Mol. weight [g/mol]: 368.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.00		Crippen Method
logp	3.787		Crippen Method
mcvol	252.260	ml/mol	McGowan Method
rinpol	2557.00		NIST Webbook
rinpol	2557.00		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=U346223&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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