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

Inchi: InChI=1S/C15H18BrNO3/c1-2-10-20-15(19)13-8-5-9-17(13)14(18)11-6-3-4-7-12(11)16/h
InchiKey: PFUPJDOVIRUJBX-UHFFFAOYSA-N
Formula: C15H18BrNO3
SMILES: CCCOC(=O)C1CCCN1C(=O)c1ccccc1Br
Mol. weight [g/mol]: 340.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.16		Crippen Method
logp	3.007		Crippen Method
mcvol	224.080	ml/mol	McGowan Method
rinpol	2358.00		NIST Webbook
rinpol	2358.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346220&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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