

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

Inchi: InChI=1S/C18H24BrNO3/c1-2-3-4-7-13-23-18(22)16-11-8-12-20(16)17(21)14-9-5-6-10-1
InchiKey: IJDCGYIRUUZGTC-UHFFFAOYSA-N
Formula: C18H24BrNO3
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)c1ccccc1Br
Mol. weight [g/mol]: 382.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.41		Crippen Method
logp	4.177		Crippen Method
mcvol	266.350	ml/mol	McGowan Method
rinpol	2661.00		NIST Webbook
rinpol	2661.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346225&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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