

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

Inchi: InChI=1S/C21H30BrNO3/c1-2-3-4-5-6-7-10-16-26-21(25)19-14-11-15-23(19)20(24)17-12
InchiKey: TVYIHIFOIFDGGDI-UHFFFAOYSA-N
Formula: C21H30BrNO3
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccccc1Br
Mol. weight [g/mol]: 424.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.67		Crippen Method
logp	5.348		Crippen Method
mcvol	308.620	ml/mol	McGowan Method
rinpol	2981.00		NIST Webbook
rinpol	2981.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346226&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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