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

Inchi: InChI=1S/C14H16BrNO3/c1-2-19-14(18)12-8-5-9-16(12)13(17)10-6-3-4-7-11(10)15/h3-4
InchiKey: PZZULNZJSRPJMA-UHFFFAOYSA-N
Formula: C14H16BrNO3
SMILES: CCOC(=O)C1CCCN1C(=O)c1ccccc1Br
Mol. weight [g/mol]: 326.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	2.617		Crippen Method
mcvol	209.990	ml/mol	McGowan Method
rinpol	2262.00		NIST Webbook
rinpol	2262.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346219&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.