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

Inchi: InChI=1S/C16H20BrNO3/c1-11(2)10-21-16(20)14-8-5-9-18(14)15(19)12-6-3-4-7-13(12)1
InchiKey: WYDXBTXJLRPQEO-UHFFFAOYSA-N
Formula: C16H20BrNO3
SMILES: CC(C)COC(=O)C1CCCN1C(=O)c1ccccc1Br
Mol. weight [g/mol]: 354.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	3.253		Crippen Method
mcvol	238.170	ml/mol	McGowan Method
rinpol	2413.00		NIST Webbook
rinpol	2413.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346221&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

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