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

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

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.17		Crippen Method
logp	4.033		Crippen Method
mcvol	266.350	ml/mol	McGowan Method
rinpol	2612.00		NIST Webbook
rinpol	2612.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346224&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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

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