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

Inchi: InChI=1S/C22H32BrNO3/c1-2-3-4-5-6-7-8-11-17-27-22(26)20-15-12-16-24(20)21(25)18-
InchiKey: FGFHODCXMIWYOO-UHFFFAOYSA-N
Formula: C22H32BrNO3
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccccc1Br
Mol. weight [g/mol]: 438.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.09		Crippen Method
logp	5.738		Crippen Method
mcvol	322.710	ml/mol	McGowan Method
rinpol	3094.00		NIST Webbook
rinpol	3094.00		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=U346227&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.