

L-Proline, N-(5-bromovaleryl)-, propyl ester

Inchi: InChI=1S/C13H22BrNO3/c1-2-10-18-13(17)11-6-5-9-15(11)12(16)7-3-4-8-14/h11H,2-10H
InchiKey: MVWRYPUMLGPPAQ-UHFFFAOYSA-N
Formula: C13H22BrNO3
SMILES: CCCOC(=O)C1CCCN1C(=O)CCCCBr
Mol. weight [g/mol]: 320.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	2.496		Crippen Method
mcvol	219.660	ml/mol	McGowan Method
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346049&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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