

d-Proline, N-methoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C14H25NO4/c1-3-4-5-6-7-11-19-13(16)12-9-8-10-15(12)14(17)18-2/h12H,3-11H
InchiKey: ZVBQTVFVXWAYQX-UHFFFAOYSA-N
Formula: C14H25NO4
SMILES: CCCCCCOC(=O)C1CCCN1C(=O)OC
Mol. weight [g/mol]: 271.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.96		Crippen Method
logp	2.731		Crippen Method
mcvol	222.120	ml/mol	McGowan Method
rinpol	1878.00		NIST Webbook
rinpol	1878.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320791&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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