

d-Proline, N-ethoxycarbonyl-, pentyl ester

Inchi: InChI=1S/C13H23NO4/c1-3-5-6-10-18-12(15)11-8-7-9-14(11)13(16)17-4-2/h11H,3-10H2
InchiKey: QVUNHSORODBDSP-UHFFFAOYSA-N
Formula: C13H23NO4
SMILES: CCCCCOC(=O)C1CCCN1C(=O)OCC
Mol. weight [g/mol]: 257.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	2.341		Crippen Method
mcvol	208.030	ml/mol	McGowan Method
rinpol	1743.00		NIST Webbook
rinpol	1743.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320835&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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<https://www.chemeo.com/cid/117-567-3/d-Proline-N-ethoxycarbonyl-pentyl-ester.pdf>

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