

d-Proline, N-isobutoxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C14H25NO4/c1-10(2)8-18-13(16)12-6-5-7-15(12)14(17)19-9-11(3)4/h10-12H,5
InchiKey: SYSVHEAIUFHSTD-UHFFFAOYSA-N
Formula: C14H25NO4
SMILES: CC(C)COC(=O)C1CCCN1C(=O)OCC(C)C
Mol. weight [g/mol]: 271.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	2.443		Crippen Method
mcvol	222.120	ml/mol	McGowan Method
rinsol	1725.00		NIST Webbook
rinsol	1725.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320803&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/123-739-5/d-Proline-N-isobutoxycarbonyl-isobutyl-ester.pdf>

Generated by Cheméo on 2024-05-01 13:57:19.133994556 +0000 UTC m=+16861088.054571871.

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