

d-Proline, n-propoxycarbonyl-, isobutyl ester

Inchi: InChI=1S/C13H23NO4/c1-4-8-17-13(16)14-7-5-6-11(14)12(15)18-9-10(2)3/h10-11H,4-9H
InchiKey: ZVEIWLSXRLJJDE-UHFFFAOYSA-N
Formula: C13H23NO4
SMILES: CCCOC(=O)N1CCCC1C(=O)OCC(C)C
Mol. weight [g/mol]: 257.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	2.197		Crippen Method
mcvol	208.030	ml/mol	McGowan Method
rinpol	1695.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320819&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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/63-484-5/d-Proline-n-propoxycarbonyl-isobutyl-ester.pdf>

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