D-Proline, N-isobutoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C17H31NO4/c1-4-5-6-7-8-12-21-16(19)15-10-9-11-18(15)17(20)22-13-14(2)3/l
InchiKey: CMKGZQWYCLLNKB-UHFFFAOYSA-N
Formula: C17H31NO4
SMILES: CCCCCCCOC(=O)C1CCCN1C(=O)OCC(C)C
Mol. weight [g/mol]: 313.44

Physical Properties

Property code	Value	Unit	Source
logp	3.757		Crippen Method
mcvol	264.390	ml/mol	McGowan Method
rinpol	2015.00		NIST Webbook
rinpol	2015.00		NIST Webbook
tb	617.11	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320807&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

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