D-Proline, N-isobutoxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C24H45NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-19-28-23(26)22-17-16-18-25(2

InchiKey: ZOWQWHJNPRPPFY-UHFFFAOYSA-N

Formula: C24H45NO4

SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCC(C)C

Mol. weight [g/mol]: 411.63

Physical Properties

Property code	Value	Unit	Source
logp	6.488		Crippen Method
mcvol	363.020	ml/mol	McGowan Method
rinpol	2618.00		NIST Webbook
rinpol	2618.00		NIST Webbook
tb	665.19	K	Cheméo Relay (1.0)

Sources

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320813&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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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