D-proline, n-isobutoxycarbonyl-, octadecyl ester

Inchi: InChI=1S/C28H53NO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-23-32-27(30)26-2

InchiKey: OGJMVABFGDCCPE-UHFFFAOYSA-N

Formula: C28H53NO4

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

Mol. weight [g/mol]: 467.73

Physical Properties

Property code	Value	Unit	Source
logp	8.048		Crippen Method
mcvol	419.380	ml/mol	McGowan Method
rinpol	3136.00		NIST Webbook
tb	690.89	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320817&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