d-Proline, n-propoxycarbonyl-, hexadecyl ester

Inchi: InChI=1S/C25H47NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-22-29-24(27)23-19-18-2

InchiKey: LJEKGBUAVPLPKU-UHFFFAOYSA-N

Formula: C25H47NO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCCC

Mol. weight [g/mol]: 425.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.57		Crippen Method
logp	7.022		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
rinpol	2794.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320831&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