D-Proline, N-propoxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C23H43NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-20-27-22(25)21-17-16-18-24(2

InchiKey: WSXKUURCVHNCHR-UHFFFAOYSA-N

Formula: C23H43NO4

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

Mol. weight [g/mol]: 397.60

Physical Properties

Property code	Value	Unit	Source
logp	6.242		Crippen Method
mcvol	348.930	ml/mol	McGowan Method
rinpol	2593.00		NIST Webbook
rinpol	2593.00		NIST Webbook
tf	307.26	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320829&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

Legend

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point

Latest version available from: