D-Proline, N-propoxycarbonyl-, heptadecyl ester

Inchi: InChI=1S/C26H49NO4/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-23-30-25(28)24-20-1

InchiKey: CJBALMNABJZTME-UHFFFAOYSA-N

Formula: C26H49NO4

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

Mol. weight [g/mol]: 439.68

Physical Properties

Property code	Value	Unit	Source
logp	7.412		Crippen Method
mcvol	391.200	ml/mol	McGowan Method
rinpol	2922.00		NIST Webbook
tf	315.99	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=U320832&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:
https://www.chemeo.com/cid/45-643-8/D-Proline-N-propoxycarbonyl-heptadecyl-ester.pdf

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