D-Proline, N-propoxycarbonyl-, heptyl ester

Inchi: InChI=1S/C16H29NO4/c1-3-5-6-7-8-13-20-15(18)14-10-9-11-17(14)16(19)21-12-4-2/h14
InchiKey: RJRFTHVMZVTNBF-UHFFFAOYSA-N
Formula: C16H29NO4
SMILES: CCCCCCCOC(=O)C1CCCN1C(=O)OCCC
Mol. weight [g/mol]: 299.41

Physical Properties

Property code	Value	Unit	Source
logp	3.511		Crippen Method
mcvol	250.300	ml/mol	McGowan Method
rinpol	1987.00		NIST Webbook
rinpol	1987.00		NIST Webbook
tf	277.61	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U320825&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
tf: Normal melting (fusion) point

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