

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]:	425.65

Physical Properties

Property code	Value	Unit	Source
logp	7.022		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
rinpol	2794.00		NIST Webbook
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tf	313.73	K	Cheméo Relay (1.0)

Sources

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