

D-Proline, N-propoxycarbonyl-, nonyl ester

Inchi:	InChI=1S/C18H33NO4/c1-3-5-6-7-8-9-10-15-22-17(20)16-12-11-13-19(16)18(21)23-14-4
InchiKey:	SFLZKSXXQIXQEI-UHFFFAOYSA-N
Formula:	C18H33NO4
SMILES:	CCCCCCCCCOC(=O)C1CCCN1C(=O)OCCC
Mol. weight [g/mol]:	327.46

Physical Properties

Property code	Value	Unit	Source
logp	4.291		Crippen Method
mcvol	278.480	ml/mol	McGowan Method
rinpol	2160.00		NIST Webbook
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tf	286.81	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320826&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):

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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<https://www.cheméo.com/cid/15-334-4/D-Proline-N-propoxycarbonyl-nonyl-ester.pdf>

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