

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:	CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OCCC
Mol. weight [g/mol]:	439.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.99		Crippen Method
logp	7.412		Crippen Method
mcvol	391.200	ml/mol	McGowan Method
rinpol	2922.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320832&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/45-643-8/d-Proline-n-propoxycarbonyl-heptadecyl-ester.pdf>

Generated by Cheméo on 2025-12-19 20:16:21.59353921 +0000 UTC m=+5923579.123579864.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.