

L-Proline, N-(cyclopropylcarbonyl)-, octadecyl ester

Inchi: InChI=1S/C27H49NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-23-31-27(30)25-19-
InchiKey: HXHYWDNPESOVBV-UHFFFAOYSA-N
Formula: C27H49NO3
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)C1CC1
Mol. weight [g/mol]: 435.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.99		Crippen Method
logp	7.192		Crippen Method
mcvol	388.560	ml/mol	McGowan Method
rinpol	3372.00		NIST Webbook
rinpol	3372.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346324&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/94-823-4/L-Proline-N-cyclopropylcarbonyl-octadecyl-ester.pdf>

Generated by Cheméo on 2025-12-23 02:27:07.932048995 +0000 UTC m=+6205025.462089650.

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