

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: CCCCCCCCOC(=O)C1CCCN1C(=O)OCCC
Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	4.291		Crippen Method
mcvol	278.480	ml/mol	McGowan Method
rinpol	2160.00		NIST Webbook
rinpol	2160.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320826&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/15-334-4/d-Proline-n-propoxycarbonyl-nonyl-ester.pdf>

Generated by Cheméo on 2024-04-19 01:50:17.512966018 +0000 UTC m=+15780666.433543330.

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