

d-Proline, N-allyloxycarbonyl-, nonyl ester

Inchi: InChI=1S/C18H31NO4/c1-3-5-6-7-8-9-10-15-22-17(20)16-12-11-13-19(16)18(21)23-14-4
InchiKey: OIBMFKYXOFQJDA-UHFFFAOYSA-N
Formula: C18H31NO4
SMILES: C=CCOC(=O)N1CCCC1C(=O)OCCCCCCCCC
Mol. weight [g/mol]: 325.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.49		Crippen Method
logp	4.067		Crippen Method
mcvol	274.180	ml/mol	McGowan Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320969&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/99-384-7/d-Proline-N-allyloxycarbonyl-nonyl-ester.pdf>

Generated by Cheméo on 2024-04-23 14:26:01.13758333 +0000 UTC m=+16171610.058160641.

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