

d-Proline, N-methoxycarbonyl-, octadecyl ester

Inchi:	InChI=1S/C25H47NO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-22-30-24(27)23-20
InchiKey:	CKZJTSNWBODILS-UHFFFAOYSA-N
Formula:	C25H47NO4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)OC
Mol. weight [g/mol]:	425.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.57		Crippen Method
logp	7.022		Crippen Method
mcvol	377.110	ml/mol	McGowan Method
rinpol	2916.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320800&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/58-290-6/d-Proline-N-methoxycarbonyl-octadecyl-ester.pdf>

Generated by Cheméo on 2024-04-25 16:43:39.361762119 +0000 UTC m=+16352668.282339431.

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