L-Proline, N-(hexanoyl)-, heptyl ester

Inchi:	InChI=1S/C18H33NO3/c1-3-5-7-8-10-15-22-18(21)16-12-11-14-19(16)17(20)13-9-6-4-2/l
InchiKey:	BVQAOYNHIKNHSE-UHFFFAOYSA-N
Formula:	C18H33NO3
SMILES:	CCCCCCCOC(=O)C1CCCN1C(=O)CCCCC
Mol. weight [g/mol]:	311.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.57		Crippen Method
logp	4.071		Crippen Method
mcvol	272.610	ml/mol	McGowan Method
rinpol	2322.00		NIST Webbook
rinpol	2322.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346157&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/97-471-2/L-Proline-N-hexanoyl-heptyl-ester.pdf
Generated by Cheméo on 2024-10-12 08:00:20.895426526 +0000 UTC m=+3300883.532395775.

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