

L-Proline, N-(1-naphthoyl)-, heptyl ester

Inchi:	InChI=1S/C23H29NO3/c1-2-3-4-5-8-17-27-23(26)21-15-10-16-24(21)22(25)20-14-9-12-1
InchiKey:	CNYADDUTDQDPME-UHFFFAOYSA-N
Formula:	C23H29NO3
SMILES:	CCCCCCCOC(=O)C1CCCN1C(=O)c1cccc2ccccc12
Mol. weight [g/mol]:	367.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.47		Crippen Method
logp	4.958		Crippen Method
mcvol	299.840	ml/mol	McGowan Method
rinpol	3067.00		NIST Webbook
rinpol	3067.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346089&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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