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

Inchi: InChI=1S/C18H19NO3/c1-2-22-18(21)16-11-6-12-19(16)17(20)15-10-5-8-13-7-3-4-9-14(
InchiKey: OPRQWQMZFGPBSP-UHFFFAOYSA-N
Formula: C18H19NO3
SMILES: CCOC(=O)C1CCCN1C(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 297.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	3.007		Crippen Method
mcvol	229.390	ml/mol	McGowan Method
rinpol	2562.00		NIST Webbook
rinpol	2562.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346082&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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