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

Inchi: InChI=1S/C20H23NO3/c1-2-3-14-24-20(23)18-12-7-13-21(18)19(22)17-11-6-9-15-8-4-5-
InchiKey: DMABAYCRXQIOIL-UHFFFAOYSA-N
Formula: C20H23NO3
SMILES: CCCCOC(=O)C1CCCN1C(=O)c1cccc2ccccc12
Mol. weight [g/mol]: 325.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.22		Crippen Method
logp	3.788		Crippen Method
mcvol	257.570	ml/mol	McGowan Method
rinpol	2752.00		NIST Webbook
rinpol	2752.00		NIST Webbook

Sources

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=U346085&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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