L-Proline, N-(furoyl-2)-, decyl ester

Inchi: InChI=1S/C20H31NO4/c1-2-3-4-5-6-7-8-9-15-25-20(23)17-12-10-14-21(17)19(22)18-13-
InchiKey: CABDCVIRZQHEBZ-UHFFFAOYSA-N
Formula: C20H31NO4
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)c1ccco1
Mol. weight [g/mol]: 349.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.66		Crippen Method
logp	4.568		Crippen Method
mcvol	287.200	ml/mol	McGowan Method
rinpol	2698.00		NIST Webbook
rinpol	2698.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U346112&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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.