L-Proline, N-(thiophen-2-carbonyl)-, dodecyl ester

Inchi: InChI=1S/C22H35NO3S/c1-2-3-4-5-6-7-8-9-10-11-17-26-22(25)19-14-12-16-23(19)21(24
InchiKey: UWXZRRHYTGBZRG-UHFFFAOYSA-N
Formula: C22H35NO3S
SMILES: CCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccs1
Mol. weight [g/mol]: 393.58

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.52		Crippen Method
logp	5.817		Crippen Method
mcvol	325.860	ml/mol	McGowan Method
rinpol	3146.00		NIST Webbook
rinpol	3146.00		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=U346378&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.