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

Inchi: InChI=1S/C21H33NO3S/c1-2-3-4-5-6-7-8-9-10-16-25-21(24)18-13-11-15-22(18)20(23)19
InchiKey: UNCNFWIUTVUFTO-UHFFFAOYSA-N
Formula: C21H33NO3S
SMILES: CCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccs1
Mol. weight [g/mol]: 379.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.10		Crippen Method
logp	5.427		Crippen Method
mcvol	311.770	ml/mol	McGowan Method
rinpol	3039.00		NIST Webbook
rinpol	3039.00		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=U346377&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

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