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

Inchi: InChI=1S/C24H39NO3S/c1-2-3-4-5-6-7-8-9-10-11-12-13-19-28-24(27)21-16-14-18-25(21

InchiKey: DDXODEDIFGHCJA-UHFFFAOYSA-N

Formula: C24H39NO3S

SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccs1

Mol. weight [g/mol]: 421.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.36		Crippen Method
logp	6.597		Crippen Method
mcvol	354.040	ml/mol	McGowan Method
rinpol	3362.00		NIST Webbook
rinpol	3362.00		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=U346379&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.