

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

Inchi: InChI=1S/C20H31NO3S/c1-2-3-4-5-6-7-8-9-15-24-20(23)17-12-10-14-21(17)19(22)18-13
InchiKey: MRAHQKHFWMTGBR-UHFFFAOYSA-N
Formula: C20H31NO3S
SMILES: CCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccs1
Mol. weight [g/mol]: 365.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.68		Crippen Method
logp	5.037		Crippen Method
mcvol	297.680	ml/mol	McGowan Method
rinpol	2912.00		NIST Webbook
rinpol	2912.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346376&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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

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