

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

Inchi: InChI=1S/C26H43NO3S/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-21-30-26(29)23-18-16-20
InchiKey: JFEQLZBFQJJHRP-UHFFFAOYSA-N
Formula: C26H43NO3S
SMILES: CCCCCCCCCCCCCCOC(=O)C1CCCN1C(=O)c1cccs1
Mol. weight [g/mol]: 449.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.20		Crippen Method
logp	7.377		Crippen Method
mcvol	382.220	ml/mol	McGowan Method
rinpol	3586.00		NIST Webbook
rinpol	3586.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346381&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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