

Sarcosine, N-(2-thienylcarbonyl)-, decyl ester

Inchi: InChI=1S/C18H29NO3S/c1-3-4-5-6-7-8-9-10-13-22-17(20)15-19(2)18(21)16-12-11-14-23
InchiKey: LTLAMNCOPFFPBX-UHFFFAOYSA-N
Formula: C18H29NO3S
SMILES: CCCCCCCCCOC(=O)CN(C)C(=O)c1cccs1
Mol. weight [g/mol]: 339.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.84		Crippen Method
logp	4.504		Crippen Method
mcvol	280.360	ml/mol	McGowan Method
rinpol	2658.00		NIST Webbook
rinpol	2658.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321471&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

Latest version available from:

<https://www.chemeo.com/cid/123-974-4/Sarcosine-N-2-thienylcarbonyl-decyl-ester.pdf>

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