

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

Inchi: InChI=1S/C16H25NO3S/c1-3-4-5-6-7-8-11-20-15(18)13-17(2)16(19)14-10-9-12-21-14/h9
InchiKey: XTAOGLWQOTXLAA-UHFFFAOYSA-N
Formula: C16H25NO3S
SMILES: CCCCCCOC(=O)CN(C)C(=O)c1cccs1
Mol. weight [g/mol]: 311.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.00		Crippen Method
logp	3.724		Crippen Method
mcvol	252.180	ml/mol	McGowan Method
rinpol	2440.00		NIST Webbook
rinpol	2440.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321469&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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<https://www.chemeo.com/cid/114-242-6/Sarcosine-N-2-thienylcarbonyl-octyl-ester.pdf>

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