

Sarcosine, N-(2-thiophenylacetyl)-, nonyl ester

Inchi: InChI=1S/C18H29NO3S/c1-3-4-5-6-7-8-9-12-22-18(21)15-19(2)17(20)14-16-11-10-13-23
InchiKey: ZGICJOINQJUIGO-UHFFFAOYSA-N
Formula: C18H29NO3S
SMILES: CCCCCCCCCOC(=O)CN(C)C(=O)Cc1cccs1
Mol. weight [g/mol]: 339.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.26		Crippen Method
logp	4.043		Crippen Method
mcvol	280.360	ml/mol	McGowan Method
rinpol	2628.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321368&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.chemeo.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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<https://www.chemeo.com/cid/49-731-6/Sarcosine-N-2-thiophenylacetyl-nonyl-ester.pdf>

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