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

Inchi: InChI=1S/C15H23NO3S/c1-3-4-5-6-9-19-15(18)12-16(2)14(17)11-13-8-7-10-20-13/h7-8,
InchiKey: YZMCWQVAJZAZQM-UHFFFAOYSA-N
Formula: C15H23NO3S
SMILES: CCCCCCOC(=O)CN(C)C(=O)Cc1cccs1
Mol. weight [g/mol]: 297.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.01		Crippen Method
logp	2.872		Crippen Method
mcvol	238.090	ml/mol	McGowan Method
rinpol	2316.00		NIST Webbook
rinpol	2316.00		NIST Webbook

Sources

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=U321365&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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