

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

Inchi:	InChI=1S/C13H19NO3S/c1-10(2)9-17-13(16)8-14(3)12(15)7-11-5-4-6-18-11/h4-6,10H,7-
InchiKey:	IHPJQNWROTXFRR-UHFFFAOYSA-N
Formula:	C13H19NO3S
SMILES:	CC(C)COC(=O)CN(C)C(=O)Cc1cccs1
Mol. weight [g/mol]:	269.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.93		Crippen Method
logp	1.948		Crippen Method
mcvol	209.910	ml/mol	McGowan Method
rinpol	2072.00		NIST Webbook
rinpol	2072.00		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=U321362&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/28-937-1/Sarcosine-N-2-thiophenylacetyl-isobutyl-ester.pdf>

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