

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

Inchi:	InChI=1S/C13H19NO3S/c1-3-4-7-17-13(16)10-14(2)12(15)9-11-6-5-8-18-11/h5-6,8H,3-4
InchiKey:	ISQNDEWDILMVQA-UHFFFAOYSA-N
Formula:	C13H19NO3S
SMILES:	CCCCOC(=O)CN(C)C(=O)Cc1cccs1
Mol. weight [g/mol]:	269.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.17		Crippen Method
logp	2.092		Crippen Method
mcvol	209.910	ml/mol	McGowan Method
rinpol	2119.00		NIST Webbook
rinpol	2119.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321363&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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