

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

Inchi:	InChI=1S/C21H35NO3S/c1-3-4-5-6-7-8-9-10-11-12-15-25-21(24)18-22(2)20(23)17-19-14
InchiKey:	QSXRHNMEFCWPRI-UHFFFAOYSA-N
Formula:	C21H35NO3S
SMILES:	CCCCCCCCCCCCOC(=O)CN(C)C(=O)Cc1cccs1
Mol. weight [g/mol]:	381.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.52		Crippen Method
logp	5.213		Crippen Method
mcvol	322.630	ml/mol	McGowan Method
rinpol	3019.00		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=U321370&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

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