

«beta»-Alanine, N-(thiophene-2-carbonyl)-, dodecyl ester

Inchi:	InChI=1S/C20H33NO3S/c1-2-3-4-5-6-7-8-9-10-11-16-24-19(22)14-15-21-20(23)18-13-12
InchiKey:	GYKCVDVWKQCLRM-UHFFFAOYSA-N
Formula:	C20H33NO3S
SMILES:	CCCCCCCCCCCCOC(=O)CCNC(=O)c1cccs1
Mol. weight [g/mol]:	367.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.30		Crippen Method
logp	5.332		Crippen Method
mcvol	308.540	ml/mol	McGowan Method
rmpol	3052.00		NIST Webbook
rmpol	3052.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U321803&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rmpol:	Non-polar retention indices

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