

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

Inchi:	InChI=1S/C18H29NO3S/c1-2-3-4-5-6-7-8-9-14-22-17(20)12-13-19-18(21)16-11-10-15-23
InchiKey:	VZABURUEAUKFMY-UHFFFAOYSA-N
Formula:	C18H29NO3S
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1cccs1
Mol. weight [g/mol]:	339.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.46		Crippen Method
logp	4.552		Crippen Method
mcvol	280.360	ml/mol	McGowan Method
rinpola	2757.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321801&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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