

2-Thiophenecarboxamide, N-tetradecyl-

Inchi:	InChI=1S/C19H33NOS/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-20-19(21)18-15-14-17-22-18/
InchiKey:	SPRVFVJXFOTPCN-UHFFFAOYSA-N
Formula:	C19H33NOS
SMILES:	CCCCCCCCCCCCCNC(=O)c1cccs1
Mol. weight [g/mol]:	323.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.02		Crippen Method
logp	6.179		Crippen Method
mcvol	287.010	ml/mol	McGowan Method
rinpola	2743.00		NIST Webbook
rinpola	2743.00		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=U407035&Units=SI

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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