2-Thiophenecarboxamide, N-octadecyl-

Inchi: InChI=1S/C23H41NOS/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-24-23(25)22-19-
InchiKey: AUTYGALMUHJVQX-UHFFFAOYSA-N
Formula: C23H41NOS
SMILES: CCCCCCCCCCCCCCCCCCNC(=O)c1cccs1
Mol. weight [g/mol]: 379.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.69		Crippen Method
logp	7.739		Crippen Method
mcvol	343.370	ml/mol	McGowan Method
rinpol	3169.00		NIST Webbook
rinpol	3169.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U407037&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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