

2-Thiophenecarboxamide, N-dodecyl-

Inchi: InChI=1S/C17H29NOS/c1-2-3-4-5-6-7-8-9-10-11-14-18-17(19)16-13-12-15-20-16/h12-13
InchiKey: MVAJYWLPFBGQRH-UHFFFAOYSA-N
Formula: C17H29NOS
SMILES: CCCCCCCCCCNC(=O)c1cccs1
Mol. weight [g/mol]: 295.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.18		Crippen Method
logp	5.399		Crippen Method
mcvol	258.830	ml/mol	McGowan Method
rinpol	2532.00		NIST Webbook
rinpol	2532.00		NIST Webbook

Sources

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=U407034&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/121-825-1/2-Thiophenecarboxamide-N-dodecyl.pdf>

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