

2-Thiophenecarboxamide, N-undecyl-

Inchi: InChI=1S/C16H27NOS/c1-2-3-4-5-6-7-8-9-10-13-17-16(18)15-12-11-14-19-15/h11-12,14
InchiKey: RRWNAJZWASDDDK-UHFFFAOYSA-N
Formula: C16H27NOS
SMILES: CCCCCCCCCCNC(=O)c1cccs1
Mol. weight [g/mol]: 281.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.76		Crippen Method
logp	5.009		Crippen Method
mcvol	244.740	ml/mol	McGowan Method
rinpol	2421.00		NIST Webbook
rinpol	2421.00		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=U407033&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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<https://www.chemeo.com/cid/117-161-3/2-Thiophenecarboxamide-N-undecyl.pdf>

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