

2-Thiophenecarboxamide, N-hexadecyl-

Inchi: InChI=1S/C21H37NOS/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-22-21(23)20-17-16-19-
InchiKey: PFEIQWCVFBJEBU-UHFFFAOYSA-N
Formula: C₂₁H₃₇NOS
SMILES: CCCCCCCCCCCCCCNC(=O)c1cccs1
Mol. weight [g/mol]: 351.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.85		Crippen Method
logp	6.959		Crippen Method
mcvol	315.190	ml/mol	McGowan Method
rinsol	2957.00		NIST Webbook
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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=U407036&Units=SI>

Legend

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

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<https://www.cheméo.com/cid/94-656-0/2-Thiophenecarboxamide-N-hexadecyl.pdf>

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