

2-Thiophenecarboxamide, N-hexyl-

Inchi: InChI=1S/C11H17NOS/c1-2-3-4-5-8-12-11(13)10-7-6-9-14-10/h6-7,9H,2-5,8H2,1H3,(H,1
InchiKey: RMKFWCHKGTGXZBU-UHFFFAOYSA-N
Formula: C11H17NOS
SMILES: CCCCCCNC(=O)c1cccs1
Mol. weight [g/mol]: 211.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.67		Crippen Method
logp	3.058		Crippen Method
mcvol	174.290	ml/mol	McGowan Method
rinpol	1883.00		NIST Webbook
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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=U407027&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/88-215-6/2-Thiophenecarboxamide-N-hexyl.pdf>

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