

2-Thiophenecarboxamide, N-heptyl-

Inchi: InChI=1S/C12H19NOS/c1-2-3-4-5-6-9-13-12(14)11-8-7-10-15-11/h7-8,10H,2-6,9H2,1H3
InchiKey: RDEFPUMRXJGWKH-UHFFFAOYSA-N
Formula: C12H19NOS
SMILES: CCCCCCNC(=O)c1cccs1
Mol. weight [g/mol]: 225.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.08		Crippen Method
logp	3.448		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
rinpol	2005.00		NIST Webbook
rinpol	2005.00		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=U407029&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

Latest version available from:

<https://www.chemeo.com/cid/85-295-1/2-Thiophenecarboxamide-N-heptyl.pdf>

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