

2-Thiophenecarboxamide, N-pentyl-N-(2-thiophenecarbonyl)-

Inchi: InChI=1S/C15H17NO2S2/c1-2-3-4-9-16(14(17)12-7-5-10-19-12)15(18)13-8-6-11-20-13/h
InchiKey: OFCLUQWUWOGCBJ-UHFFFAOYSA-N
Formula: C15H17NO2S2
SMILES: CCCCCN(C(=O)c1cccs1)C(=O)c1cccs1
Mol. weight [g/mol]: 307.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	4.282		Crippen Method
mcvol	229.110	ml/mol	McGowan Method
rinpole	2367.00		NIST Webbook
rinpole	2367.00		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=U407040&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
rinpole: Non-polar retention indices

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