

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

Inchi: InChI=1S/C19H25NO2S2/c1-2-3-4-5-6-7-8-13-20(18(21)16-11-9-14-23-16)19(22)17-12-1
InchiKey: YIULLKJQHLTUHB-UHFFFAOYSA-N
Formula: C19H25NO2S2
SMILES: CCCCCCCCN(C(=O)c1cccs1)C(=O)c1cccs1
Mol. weight [g/mol]: 363.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.45		Crippen Method
logp	5.843		Crippen Method
mcvol	285.470	ml/mol	McGowan Method
rinpole	2801.00		NIST Webbook
rinpole	2801.00		NIST Webbook

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=U407045&Units=SI>

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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