

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

Inchi: InChI=1S/C18H23NO2S2/c1-2-3-4-5-6-7-12-19(17(20)15-10-8-13-22-15)18(21)16-11-9-1
InchiKey: KRSXWWXGZFJEMF-UHFFFAOYSA-N
Formula: C18H23NO2S2
SMILES: CCCCCCN(C(=O)c1cccs1)C(=O)c1cccs1
Mol. weight [g/mol]: 349.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.03		Crippen Method
logp	5.453		Crippen Method
mcvol	271.380	ml/mol	McGowan Method
rinpola	2685.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U407044&Units=SI>

Legend

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

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