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

Inchi: InChI=1S/C17H21NO2S2/c1-2-3-4-5-6-11-18(16(19)14-9-7-12-21-14)17(20)15-10-8-13-2
InchiKey: JWMWWLAQLBPZQO-UHFFFAOYSA-N
Formula: C17H21NO2S2
SMILES: CCCCCCCN(C(=O)c1cccs1)C(=O)c1cccs1
Mol. weight [g/mol]: 335.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.61		Crippen Method
logp	5.063		Crippen Method
mcvol	257.290	ml/mol	McGowan Method
rinpol	2581.00		NIST Webbook
rinpol	2581.00		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=U407043&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.