

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

Inchi: InChI=1S/C18H23NO2S2/c1-3-5-8-14(4-2)13-19(17(20)15-9-6-11-22-15)18(21)16-10-7-1
InchiKey: FNACHQFJMHNDK-UHFFFAOYSA-N
Formula: C18H23NO2S2
SMILES: CCCCC(CC)CN(C(=O)c1cccs1)C(=O)c1cccs1
Mol. weight [g/mol]: 349.51

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.79 | | Crippen Method |
| logp | 5.309 | | Crippen Method |
| mcvol | 271.380 | ml/mol | McGowan Method |
| rmpol | 2558.00 | | NIST Webbook |
| rmpol | 2558.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U407042&Units=SI>
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>

Legend

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

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