

Thiophene-2-carboxamide, N,N-dihexyl-

Inchi: InChI=1S/C17H29NOS/c1-3-5-7-9-13-18(14-10-8-6-4-2)17(19)16-12-11-15-20-16/h11-12
InchiKey: DEMCLDOPCCTVHO-UHFFFAOYSA-N
Formula: C17H29NOS
SMILES: CCCCCCN(CCCCC)C(=O)c1cccs1
Mol. weight [g/mol]: 295.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.56		Crippen Method
logp	5.351		Crippen Method
mcvol	258.830	ml/mol	McGowan Method
rinpola	2201.00		NIST Webbook
rinpola	2201.00		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=U308192&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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