

Thiophene-2-carboxamide, N,N-diundecyl-

Inchi: InChI=1S/C27H49NOS/c1-3-5-7-9-11-13-15-17-19-23-28(27(29)26-22-21-25-30-26)24-2
InchiKey: AZDRLYBCCZOHEU-UHFFFAOYSA-N
Formula: C27H49NOS
SMILES: CCCCCCCCCCN(CCCCCCCCCC)C(=O)c1cccs1
Mol. weight [g/mol]: 435.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.74		Crippen Method
logp	9.252		Crippen Method
mcvol	399.730	ml/mol	McGowan Method
rinpole	3417.00		NIST Webbook
rinpole	3417.00		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=U308200&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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