

Thiophene-2-carboxamide, N,N-diheptyl-

Inchi: InChI=1S/C19H33NOS/c1-3-5-7-9-11-15-20(16-12-10-8-6-4-2)19(21)18-14-13-17-22-18/
InchiKey: WEZSCFLGRFFMGD-UHFFFAOYSA-N
Formula: C19H33NOS
SMILES: CCCCCCN(CCCCCC)C(=O)c1cccs1
Mol. weight [g/mol]: 323.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.40		Crippen Method
logp	6.131		Crippen Method
mcvol	287.010	ml/mol	McGowan Method
rinpol	2406.00		NIST Webbook
rinpol	2406.00		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=U308195&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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<https://www.chemeo.com/cid/99-577-3/Thiophene-2-carboxamide-N-N-diheptyl.pdf>

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