

Thiophene-2-carboxamide, N-ethyl-N-octadecyl-

Inchi: InChI=1S/C25H45NOS/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-26(4-2)25(27)
InchiKey: RXAZHABTQVRTGS-UHFFFAOYSA-N
Formula: C25H45NOS
SMILES: CCCCCCCCCCCCCCCCCCN(CC)C(=O)c1cccs1
Mol. weight [g/mol]: 407.70

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.91		Crippen Method
logp	8.472		Crippen Method
mcvol	371.550	ml/mol	McGowan Method
rinpol	1775.00		NIST Webbook
rinpol	1775.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U415318&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.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
rinpol: Non-polar retention indices

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