

Thiophene-2-carboxamide, N-ethyl-N-hexadecyl-

Inchi: InChI=1S/C23H41NOS/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17-20-24(4-2)23(25)22-19-
InchiKey: AOSSQHBVVIVYOB-UHFFFAOYSA-N
Formula: C23H41NOS
SMILES: CCCCCCCCCCCCCCN(CC)C(=O)c1cccs1
Mol. weight [g/mol]: 379.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.07		Crippen Method
logp	7.692		Crippen Method
mcvol	343.370	ml/mol	McGowan Method
rinsol	1729.00		NIST Webbook
rinsol	1729.00		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=U415317&Units=SI>

Legend

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

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