

Thiophene-2-carboxamide, N-ethyl-N-heptyl-

Inchi: InChI=1S/C14H23NOS/c1-3-5-6-7-8-11-15(4-2)14(16)13-10-9-12-17-13/h9-10,12H,3-8,1
InchiKey: RRZCXFAMMQAMLK-UHFFFAOYSA-N
Formula: C14H23NOS
SMILES: CCCCCCN(CC)C(=O)c1cccs1
Mol. weight [g/mol]: 253.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.30		Crippen Method
logp	4.181		Crippen Method
mcvol	216.560	ml/mol	McGowan Method
rinpol	2216.00		NIST Webbook
rinpol	2216.00		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=U415310&Units=SI>

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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