Thiophene-2-carboxamide, N-(1-naphthyl)-

Inchi: InChI=1S/C15H11NOS/c17-15(14-9-4-10-18-14)16-13-8-3-6-11-5-1-2-7-12(11)13/h1-10H
InchiKey: AKWLMJIIXUBZSM-UHFFFAOYSA-N
Formula: C15H11NOS
SMILES: O=C(Nc1cccc2ccccc12)c1cccs1
Mol. weight [g/mol]: 253.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.01		Crippen Method
logp	4.154		Crippen Method
mcvol	187.430	ml/mol	McGowan Method
rinpol	2498.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307076&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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