Thiophene-2-carboxamide, N-ethyl-N-(3-methylphenyl)-

Inchi: InChI=1S/C14H15NOS/c1-3-15(12-7-4-6-11(2)10-12)14(16)13-8-5-9-17-13/h4-10H,3H2,1
InchiKey: YFJNAIMKFSZOKA-UHFFFAOYSA-N
Formula: C14H15NOS
SMILES: CCN(C(=O)c1cccs1)c1cccc(C)c1
Mol. weight [g/mol]: 245.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.00		Crippen Method
logp	3.723		Crippen Method
mcvol	192.800	ml/mol	McGowan Method
rinpol	1917.00		NIST Webbook
rinpol	1917.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U308191&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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