2-Thiopheneacetamide, N-ethyl-N-(3-methylphenyl)-

Inchi: InChI=1S/C15H17NOS/c1-3-16(13-7-4-6-12(2)10-13)15(17)11-14-8-5-9-18-14/h4-10H,3,

InchiKey: VFROVHWHIVARFH-UHFFFAOYSA-N

Formula: C15H17NOS

SMILES: CCN(C(=O)Cc1cccs1)c1cccc(C)c1

Mol. weight [g/mol]: 259.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	3.652		Crippen Method
mcvol	206.890	ml/mol	McGowan Method
rinpol	1997.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U308136&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