

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

Inchi: InChI=1S/C12H11NOS/c1-9-4-2-5-10(8-9)13-12(14)11-6-3-7-15-11/h2-8H,1H3,(H,13,14)
InchiKey: LNBFMVUOGDNKPI-UHFFFAOYSA-N
Formula: C12H11NOS
SMILES: Cc1cccc(NC(=O)c2cccs2)c1
Mol. weight [g/mol]: 217.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.68		Crippen Method
logp	3.309		Crippen Method
mcvol	164.620	ml/mol	McGowan Method
rinsol	2037.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=U307069&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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<https://www.chemeo.com/cid/85-599-4/Thiophene-2-carboxamide-N-3-methylphenyl.pdf>

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