

N-(4-Methoxyphenyl)-thiophene-2-carboxamide

Other names: Thiophene-2-carboxamide, N-(4-methoxyphenyl)-
Inchi: InChI=1S/C12H11NO2S/c1-15-10-6-4-9(5-7-10)13-12(14)11-3-2-8-16-11/h2-8H,1H3,(H,1
InchiKey: DTHZTXGJRSLGFS-UHFFFAOYSA-N
Formula: C12H11NO2S
SMILES: COc1ccc(NC(=O)c2cccs2)cc1
Mol. weight [g/mol]: 233.29
CAS: 64419-14-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Crippen Method
logp	3.009		Crippen Method
mcvol	170.490	ml/mol	McGowan Method
rinpol	2217.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C64419143&Units=SI>
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>

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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