

Thiophene-2-carboxamide, N-(4-fluorophenyl)-

Inchi: InChI=1S/C11H8FNOS/c12-8-3-5-9(6-4-8)13-11(14)10-2-1-7-15-10/h1-7H,(H,13,14)
InchiKey: GCPZKCOCHNSMRNY-UHFFFAOYSA-N
Formula: C11H8FNOS
SMILES: O=C(Nc1ccc(F)cc1)c1cccs1
Mol. weight [g/mol]: 221.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	3.139		Crippen Method
mcvol	152.300	ml/mol	McGowan Method
rinpol	1926.00		NIST Webbook
rinpol	1926.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307068&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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<https://www.chemeo.com/cid/112-707-2/Thiophene-2-carboxamide-N-4-fluorophenyl.pdf>

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