

Isonicotinamide, N-(4-fluorophenyl)-

Inchi: InChI=1S/C12H9FN2O/c13-10-1-3-11(4-2-10)15-12(16)9-5-7-14-8-6-9/h1-8H,(H,15,16)
InchiKey: WSJKQVNRSGJES-UHFFFAOYSA-N
Formula: C12H9FN2O
SMILES: O=C(Nc1ccc(F)cc1)c1ccncc1
Mol. weight [g/mol]: 216.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.54		Crippen Method
logp	2.473		Crippen Method
mcvol	155.720	ml/mol	McGowan Method
rinpol	1942.00		NIST Webbook
rinpol	1942.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U307412&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/125-044-4/Isonicotinamide-N-4-fluorophenyl.pdf>

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