

Isonicotinic acid, morpholide

Inchi: InChI=1S/C10H12N2O2/c13-10(9-1-3-11-4-2-9)12-5-7-14-8-6-12/h1-4H,5-8H2
InchiKey: LKCRGBNWPDHINV-UHFFFAOYSA-N
Formula: C10H12N2O2
SMILES: O=C(c1ccncc1)N1CCOCC1
Mol. weight [g/mol]: 192.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.20		Crippen Method
logp	0.554		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
rmpol	1703.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=U307411&Units=SI>

Legend

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

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<https://www.cheméo.com/cid/125-047-1/Isonicotinic-acid-morpholide.pdf>

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