

# Isonicotinamide, N-(4-bromophenyl)-

**Inchi:** InChI=1S/C12H9BrN2O/c13-10-1-3-11(4-2-10)15-12(16)9-5-7-14-8-6-9/h1-8H,(H,15,16)  
**InchiKey:** GGRSQUETTIVASD-UHFFFAOYSA-N  
**Formula:** C12H9BrN2O  
**SMILES:** O=C(Nc1ccc(Br)cc1)c1cncc1  
**Mol. weight [g/mol]:** 277.12

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.38		Crippen Method
logp	3.096		Crippen Method
mcvol	171.450	ml/mol	McGowan Method
rinpola	2278.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=U307415&Units=SI>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/61-173-2/Isonicotinamide-N-4-bromophenyl.pdf>

Generated by Cheméo on 2024-04-19 17:30:20.911434023 +0000 UTC m=+15837069.832011345.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.