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: GGRSQPUETTVASD-UHFFFAOYSA-N
Formula: C12H9BrN2O
SMILES: O=C(Nc1ccc(Br)cc1)c1ccncc1
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
rinpol	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
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
rinpol: Non-polar retention indices