

Nicotinamide, N-(4-bromophenyl)-

Inchi: InChI=1S/C12H9BrN2O/c13-10-3-5-11(6-4-10)15-12(16)9-2-1-7-14-8-9/h1-8H,(H,15,16)
InchiKey: ZSPAJDNLIXHAD-UHFFFAOYSA-N
Formula: C12H9BrN2O
SMILES: O=C(Nc1ccc(Br)cc1)c1cccnc1
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	2311.00		NIST Webbook
rinpol	2311.00		NIST Webbook

Sources

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=U308108&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/118-442-0/Nicotinamide-N-4-bromophenyl.pdf>

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