

# Methanone, (2-amino-5-bromophenyl)-2-pyridinyl-

<b>Other names:</b>	2-(2'-Amino-5'-bromobenzoyl)pyridine 2-(2-Amino-5-brom-benzoyl)-pyridine 2-(2-Amino-5-bromobenzoyl)-pyridine Pyridine, 2-(2-amino-5-bromobenzoyl) Bromazepam benzophenone 2-amino-5-bromobenzoylpyridine
<b>Inchi:</b>	InChI=1S/C12H9BrN2O/c13-8-4-5-10(14)9(7-8)12(16)11-3-1-2-6-15-11/h1-7H,14H2
<b>InchiKey:</b>	KHVZPFKJBLTYCC-UHFFFAOYSA-N
<b>Formula:</b>	C12H9BrN2O
<b>SMILES:</b>	<chem>Nc1ccc(Br)cc1C(=O)c1ccccn1</chem>
<b>Mol. weight [g/mol]:</b>	277.12
<b>CAS:</b>	1563-56-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	2.657		Crippen Method
mcvol	171.450	ml/mol	McGowan Method
rinpol	2240.00		NIST Webbook
rinpol	2277.00		NIST Webbook
rinpol	2259.00		NIST Webbook
rinpol	2240.00		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C1563560&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1563560&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

# Legend

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

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