

# brompyrazone

<b>Other names:</b>	5-amino-4-bromo-2-phenylpyridazin-3-one
<b>Inchi:</b>	InChI=1S/C10H8BrN3O/c11-9-8(12)6-13-14(10(9)15)7-4-2-1-3-5-7/h1-6H,12H2
<b>InchiKey:</b>	ODNZLRLWXRXPOH-UHFFFAOYSA-N
<b>Formula:</b>	C10H8BrN3O
<b>SMILES:</b>	<chem>Nc1cnn(-c2ccccc2)c(=O)c1Br</chem>
<b>Mol. weight [g/mol]:</b>	266.10

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Aqueous Solubility Prediction Method
log10ws	-3.13		Estimated Solubility Method
logp	1.577		Crippen Method
mcvol	157.550	ml/mol	McGowan Method
tf	496.65	K	Aqueous Solubility Prediction Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

**Estimated Solubility Method:** [http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)

## 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>tf:</b>	Normal melting (fusion) point

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