2-Amino-5-bromo-3-nitropyridine

Other names:	2-Pyridinamine, 5-bromo-3-nitro-
Inchi:	InChI=1S/C5H4BrN3O2/c6-3-1-4(9(10)11)5(7)8-2-3/h1-2H,(H2,7,8)
InchiKey:	QOOCOFOGYRQPPN-UHFFFAOYSA-N
Formula:	C5H4BrN3O2
SMILES:	Nc1ncc(Br)cc1[N+](=O)[O-]
Mol. weight [g/mol]:	218.01
CAS:	6945-68-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.68		Crippen Method
logp	1.335		Crippen Method
mcvol	112.430	ml/mol	McGowan Method

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=C6945682&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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