

3-Pyridinol, 2-bromo-

Other names:	2-Bromo-3-hydroxypyridine 2-Bromo-3-pyridinol 2-bromopyridin-3-ol
Inchi:	InChI=1S/C5H4BrNO/c6-5-4(8)2-1-3-7-5/h1-3,8H
InchiKey:	YKHQFTANTNMYPP-UHFFFAOYSA-N
Formula:	C5H4BrNO
SMILES:	Oc1cccnc1Br
Mol. weight [g/mol]:	174.00
CAS:	6602-32-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.95		Crippen Method
logp	1.550		Crippen Method
mcvol	90.900	ml/mol	McGowan Method

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=C6602320&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/96-765-7/3-Pyridinol-2-bromo.pdf>

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