

3-Amino-4-bromopyrazole

Inchi:	InChI=1S/C3H4BrN3/c4-2-1-6-7-3(2)5/h1H,(H3,5,6,7)
InchiKey:	OELYMZVJDKSMOJ-UHFFFAOYSA-N
Formula:	C3H4BrN3
SMILES:	Nc1[nH]ncc1Br
Mol. weight [g/mol]:	161.99
CAS:	16461-94-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.25		Crippen Method
logp	0.273		Crippen Method
mcvol	81.110	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=C16461942&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

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