

2-Amino-3-bromo-5-methylpyridine

Inchi:	InChI=1S/C6H7BrN2/c1-4-2-5(7)6(8)9-3-4/h2-3H,1H3,(H2,8,9)
InchiKey:	NDPKXEWDWTZBDG-UHFFFAOYSA-N
Formula:	C6H7BrN2
SMILES:	Cc1cnc(N)c(Br)c1
Mol. weight [g/mol]:	187.04
CAS:	17282-00-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	1.735		Crippen Method
mcvol	109.100	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C17282007&Units=SI

Legend

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

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