

4-Bromopyridine

Other names:	Pyridine, 4-bromo-
Inchi:	InChI=1S/C5H4BrN/c6-5-1-3-7-4-2-5/h1-4H
InchiKey:	BSDGZUDFPKIYQG-UHFFFAOYSA-N
Formula:	C5H4BrN
SMILES:	Brc1ccncc1
Mol. weight [g/mol]:	158.00
CAS:	1120-87-2

Physical Properties

Property code	Value	Unit	Source
affp	917.80	kJ/mol	NIST Webbook
basg	886.00	kJ/mol	NIST Webbook
ie	10.00 ± 0.10	eV	NIST Webbook
ie	9.94 ± 0.05	eV	NIST Webbook
log10ws	-2.40		Crippen Method
logp	1.844		Crippen Method
mcvol	85.030	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	302.20	K	0.05	NIST Webbook

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=C1120872&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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