

3-Amino-4-picoline

Other names:	3-Pyridinamine, 4-methyl- 4-Picoline, 3-amino-
Inchi:	InChI=1S/C6H8N2/c1-5-2-3-8-4-6(5)7/h2-4H,7H2,1H3
InchiKey:	IBKMZYWDWWIWEL-UHFFFAOYSA-N
Formula:	C6H8N2
SMILES:	Cc1ccncc1N
Mol. weight [g/mol]:	108.14
CAS:	3430-27-1

Physical Properties

Property code	Value	Unit	Source
ie	9.30	eV	NIST Webbook
log10ws	-1.35		Crippen Method
logp	0.972		Crippen Method
mcvol	91.600	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	527.20	K	98.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3430271&Units=SI
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

Legend

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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