3-Pyridinemethanamine

Other names:	Picolamine
	Pyridine, 3-(aminomethyl)-
	3-(Aminomethyl)pyridine
	3-Picolylamine
	3-Pyridinemethylamine
	NSC 59706
Inchi:	InChI=1S/C6H8N2/c7-4-6-2-1-3-8-5-6/h1-3,5H,4,7H2
InchiKey:	HDOUGSFASVGDCS-UHFFFAOYSA-N
Formula:	C6H8N2
SMILES:	NCc1cccnc1
Mol. weight [g/mol]:	108.14
CAS:	3731-52-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.55		Crippen Method
logp	0.540		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
rinpol	1066.40		NIST Webbook
rinpol	1117.00		NIST Webbook
ripol	1849.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	346.70	K	0.10	NIST Webbook
tbrp	385.00	K	2.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3731520&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tbrp:	Boiling point at reduced pressure