3-AMINO-4-PYRAZOLECARBONITRILE

Other names:	1H-Pyrazole-4-carbonitrile, 3-amino-
	3-Amino-1H-pyrazole-4-carbonitrile
	3-Amino-4-cyano-1H-pyrazole
	3-Amino-4-cyanopyrazole
	3-Aminopyrazole-4-carbonitrile
	3-Aminopyrazole-4-nitrile
	5-Amino-4-cyanopyrazole
	5-Amino-4-pyrazolecarbonitrile
	5-aminopyrazole-4-carbonitrile
	NSC 44932
	Pyrazole-4-carbonitrile, 3-amino-
Inchi:	InChI=1S/C4H4N4/c5-1-3-2-7-8-4(3)6/h2H,(H3,6,7,8)
InchiKey:	FFNKBQRKZRMYCL-UHFFFAOYSA-N
Formula:	C4H4N4
SMILES:	N#Cc1c[nH]nc1N
Mol. weight [g/mol]:	108.10

Physical Properties

Property code	Value	Unit	Source
logp	-0.618		Crippen Method
mcvol	79.080	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16617462&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume