

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:	FFNKBQRKZRMVCL-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.cheméo.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

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