

3-Aminopyrazole

Other names:	1H-Pyrazol-3-amine pyrazol-3-ylamine 3(5)-aminopyrazole
Inchi:	InChI=1S/C3H5N3/c4-3-1-2-5-6-3/h1-2H,(H3,4,5,6)
InchiKey:	JVVRJMXHNUAPHW-UHFFFAOYSA-N
Formula:	C3H5N3
SMILES:	N=c1cc[nH][nH]1
Mol. weight [g/mol]:	83.09
CAS:	1820-80-0

Physical Properties

Property code	Value	Unit	Source
affp	921.50	kJ/mol	NIST Webbook
basg	889.60	kJ/mol	NIST Webbook
log10ws	-0.90		Crippen Method
logp	-1.142		Crippen Method
mcvol	63.610	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	491.20	K	16.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1820800&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

affp:	Proton affinity
basg:	Gas basicity
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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