1-methyl-5-aminopyrazole

Inchi:	InChI=1S/C4H7N3/c1-7-4(5)2-3-6-7/h2-3H,5H2,1H3
InchiKey:	JESRNIJXVIFVOV-UHFFFAOYSA-N
Formula:	C4H7N3
SMILES:	Cn1nccc1N
Mol. weight [g/mol]:	97.12
CAS:	1192-21-8

Physical Properties

Property code	Value	Unit	Source
affp	949.50	kJ/mol	NIST Webbook
basg	917.60	kJ/mol	NIST Webbook
log10ws	-2.16		Crippen Method
logp	0.002		Crippen Method
mcvol	77.700	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1192218&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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