

1-(3-Aminopropyl)imidazole

Other names:	N-(3-Aminopropyl)imidazole 1H-Imidazole-1-propanamine 1H-imidazole-1-propylamine
Inchi:	InChI=1S/C6H11N3/c7-2-1-4-9-5-3-8-6-9/h3,5-6H,1-2,4,7H2
InchiKey:	KDHWOCLBMVSZPG-UHFFFAOYSA-N
Formula:	C6H11N3
SMILES:	NCCCN1ccnc1
Mol. weight [g/mol]:	125.17
CAS:	5036-48-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.35		Crippen Method
logp	0.232		Crippen Method
mcvol	105.880	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=C5036486&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/61-711-4/1-3-Aminopropyl-imidazole.pdf>

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