

5-Aminoindole

Other names:	1H-Indol-5-amine Indole, 5-amino- indol-5-ylamine
Inchi:	InChI=1S/C8H8N2/c9-7-1-2-8-6(5-7)3-4-10-8/h1-5,10H,9H2
InchiKey:	ZCBIFHNDZBSCEP-UHFFFAOYSA-N
Formula:	C8H8N2
SMILES:	Nc1ccc2[nH]ccc2c1
Mol. weight [g/mol]:	132.16
CAS:	5192-03-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	1.268		Crippen Method
mcvol	104.620	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5192030&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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