3-Amino-4,5-dihydro-1-phenylpyrazole

Other names:	1H-Pyrazol-3-amine, 4,5-dihydro-1-phenyl-
	Pyrazolidine, 3-imino-1-phenyl-
	1-Fenyl-3-aminopyrazolin
	2-Pyrazoline, 3-amino-1-phenyl-
	3-Amino-1-phenylpyrazole
	3-Amino-1-fenyl-2-pyrazolin
	3-Amino-1-phenyl-2-pyrazoline
	1-Phenyl-3-amino-2-pyrazoline
	3-Amino-1-phenylpyrazoline
	NSC 162874
	4,5-dihydro-1-phenyl-1H-pyrazol-3-amine
Inchi:	InChI=1S/C9H11N3/c10-9-6-7-12(11-9)8-4-2-1-3-5-8/h1-5H,6-7H2,(H2,10,11)
InchiKey:	QENUTIJJGGTTPE-UHFFFAOYSA-N
Formula:	C9H11N3
SMILES:	NC1=NN(c2ccccc2)CC1
Mol. weight [g/mol]:	161.20
CAS:	3314-35-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.78		Crippen Method
logp	1.169		Crippen Method
mcvol	128.690	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3314350&Units=SI

Legend

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