

3-Amino-1-phenyl-2-pyrazolin-5-one

Other names:	3H-Pyrazol-3-one, 5-amino-2,4-dihydro-2-phenyl-1-Phenyl-3-amino-4,5-dihydropyrazol-5-on 3-amino-1-phenyl-5-pyrazolone
Inchi:	InChI=1S/C9H9N3O/c10-8-6-9(13)12(11-8)7-4-2-1-3-5-7/h1-5H,6H2,(H2,10,11)
InchiKey:	LPOVZHYARSAVIZ-UHFFFAOYSA-N
Formula:	C9H9N3O
SMILES:	NC1=NN(c2ccccc2)C(=O)C1
Mol. weight [g/mol]:	175.19
CAS:	4149-06-8

Physical Properties

Property code	Value	Unit	Source
ie	7.40	eV	NIST Webbook
ie	7.70	eV	NIST Webbook
log10ws	-1.55		Crippen Method
logp	0.696		Crippen Method
mcvol	130.260	ml/mol	McGowan Method

Sources

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=C4149068&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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