5-Amino-3-phenylpyrazole

Other names:	3-Phenyl-1H-pyrazol-5-amine
Inchi:	InChI=1S/C9H9N3/c10-9-6-8(11-12-9)7-4-2-1-3-5-7/h1-6H,(H3,10,11,12)
InchiKey:	PWSZRRFDVPMZGM-UHFFFAOYSA-N
Formula:	C9H9N3
SMILES:	Nc1cc(-c2ccccc2)n[nH]1
Mol. weight [g/mol]:	159.19
CAS:	827-41-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	1.177		Crippen Method
mcvol	124.390	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=C827418&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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