

5-Amino-1-methyl-3-phenylpyrazole

Inchi:	InChI=1S/C10H11N3/c1-13-10(11)7-9(12-13)8-5-3-2-4-6-8/h2-7H,11H2,1H3
InchiKey:	KCYRMURRLLYLPU-UHFFFAOYSA-N
Formula:	C10H11N3
SMILES:	Cn1nc(-c2ccccc2)cc1N
Mol. weight [g/mol]:	173.21
CAS:	10199-50-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.76		Crippen Method
logp	1.669		Crippen Method
mcvol	138.480	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=C10199505&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

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