5-Amino-4-cyano-1-phenylpyrazole

Other names:	5-Amino-1-phenylpyrazole-4-carbonitrile 1H-Pyrazole-4-carbonitrile, 5-amino-1-phenyl- 5-amino-1-phenyl-1H-pyrazole-4-carbonitrile
Inchi:	InChI=1S/C10H8N4/c11-6-8-7-13-14(10(8)12)9-4-2-1-3-5-9/h1-5,7H,12H2
InchiKey:	MAKQREKUUHPPIS-UHFFFAOYSA-N
Formula:	C10H8N4
SMILES:	N#Cc1cnn(-c2ccccc2)c1N
Mol. weight [g/mol]:	184.20
CAS:	5334-43-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	1.326		Crippen Method
mcvol	139.860	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=C5334430&Units=SI

Legend

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

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