1H-Pyrazol-5-amine, 3-methyl-1-phenyl-

Other names:	1-Phenyl-3-methyl-5-aminopyrazole
	1H-Pyrazole-5-amine, 3-methyl-1-phenyl-
	3-Methyl-1-phenyl-1H-pyrazol-5-amine
	3-methyl-1-phenylpyrazol-5-ylamine
	5-Amino-3-methyl-1-phenylpyrazole
	5-methyl-2-phenylpyrazol-3-amine
	Pyrazole, 5-amino-3-methyl-1-phenyl-
Inchi:	InChI=1S/C10H11N3/c1-8-7-10(11)13(12-8)9-5-3-2-4-6-9/h2-7H,11H2,1H3
InchiKey:	FMKMKBLHMONXJM-UHFFFAOYSA-N
Formula:	C10H11N3
SMILES:	Cc1cc(N)n(-c2ccccc2)n1
Mol. weight [g/mol]:	173.21
CAS:	1131-18-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.94		Aqueous Solubility Prediction Method
logp	1.763		Crippen Method
mcvol	138.480	ml/mol	McGowan Method
tb	606.20	K	NIST Webbook
tf	389.00	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	470.20	K	2.10	NIST Webbook
tbrp	606.00	K	101.00	NIST Webbook
tbrp	470.00	K	2.10	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1131186&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point