1H-Pyrazole, 3-methyl-5-phenyl-

Other names:	Pyrazole, 3-methyl-5-phenyl-
	Femerazol
	Phemerazole
	3-Methyl-5-phenylpyrazole
	5-Methyl-3-phenylpyrazole
	3(5)-Methyl-5(3)-phenylpyrazole
	3-methyl-5-phenyl-1H-pyrazole
Inchi:	InChI=1S/C10H10N2/c1-8-7-10(12-11-8)9-5-3-2-4-6-9/h2-7H,1H3,(H,11,12)
InchiKey:	QHRSESMSOJZMCO-UHFFFAOYSA-N
Formula:	C10H10N2
SMILES:	Cc1cc(-c2ccccc2)[nH]n1
Mol. weight [g/mol]:	158.20
CAS:	3347-62-4

Physical Properties

Property code	Value	Unit	Source
affp	932.10	kJ/mol	NIST Webbook
basg	900.20	kJ/mol	NIST Webbook
log10ws	-3.54		Crippen Method
logp	1.903		Crippen Method
mcvol	128.500	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=C3347624&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume