

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

Other names:	Pyrazole, 5-methyl-1-phenyl- 1-Phenyl-5-methylpyrazole 3-Methyl-2-phenylpyrazole 5-Methyl-1-phenylpyrazole
Inchi:	InChI=1S/C10H10N2/c1-9-7-8-11-12(9)10-5-3-2-4-6-10/h2-8H,1H3
InchiKey:	GIPOQOUSJKAZMC-UHFFFAOYSA-N
Formula:	C10H10N2
SMILES:	Cc1ccnn1-c1ccccc1
Mol. weight [g/mol]:	158.20
CAS:	6831-91-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Crippen Method
logp	2.181		Crippen Method
mcvol	128.500	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	536.70	K	102.00	NIST Webbook
tbrp	417.70	K	2.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6831910&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure

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