

1H-Pyrazole, 1-phenyl-

Other names:	Pyrazole, 1-phenyl- N-Phenylpyrazole 1-Phenylpyrazole 1-Phenyl-1H-pyrazole
Inchi:	InChI=1S/C9H8N2/c1-2-5-9(6-3-1)11-8-4-7-10-11/h1-8H
InchiKey:	WITMXBRCQWOZPX-UHFFFAOYSA-N
Formula:	C9H8N2
SMILES:	<chem>c1ccc(-n2cccn2)cc1</chem>
Mol. weight [g/mol]:	144.17
CAS:	1126-00-7

Physical Properties

Property code	Value	Unit	Source
hvap	70.20 ± 3.40	kJ/mol	NIST Webbook
log10ws	-2.89		Crippen Method
logp	1.872		Crippen Method
mvol	114.410	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	414.70	K	4.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1126007&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

hvap:	Enthalpy of vaporization at standard conditions
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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