

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

Other names:	1-Methyl-3-phenylpyrazole
Inchi:	InChI=1S/C10H10N2/c1-12-8-7-10(11-12)9-5-3-2-4-6-9/h2-8H,1H3
InchiKey:	AQQUNJMVAKJGKR-UHFFFAOYSA-N
Formula:	C10H10N2
SMILES:	Cn1ccc(-c2ccccc2)n1
Mol. weight [g/mol]:	158.20
CAS:	3463-26-1

Physical Properties

Property code	Value	Unit	Source
affp	932.60	kJ/mol	NIST Webbook
basg	900.80	kJ/mol	NIST Webbook
log10ws	-5.13		Crippen Method
logp	2.087		Crippen Method
mcvol	128.500	ml/mol	McGowan Method
tb	553.70	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	411.70	K	1.60	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3463261&Units=SI

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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