1H-Pyrazole, 3-phenyl-

Other names:	Pyrazole, 3-phenyl-
	3-Phenylpyrazole
	5-Amino-3-phenylpyrazole
	3(5)-phenylpyrazole
Inchi:	InChI=1S/C9H8N2/c1-2-4-8(5-3-1)9-6-7-10-11-9/h1-7H,(H,10,11)
InchiKey:	OEDUIFSDODUDRK-UHFFFAOYSA-N
Formula:	C9H8N2
SMILES:	c1ccc(-c2cc[nH]n2)cc1
Mol. weight [g/mol]:	144.17
CAS:	2458-26-6

Physical Properties

Property code	Value	Unit	Source
affp	914.20	kJ/mol	NIST Webbook
basg	882.30	kJ/mol	NIST Webbook
log10ws	-3.06		Crippen Method
logp	1.595		Crippen Method
mcvol	114.410	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=C2458266&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

Latest version available from:

https://www.chemeo.com/cid/47-778-7/1H-Pyrazole-3-phenyl.pdf

Generated by Cheméo on 2024-10-12 02:54:24.909102131 +0000 UTC m=+3282527.546071382.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.