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: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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