1H-Pyrazole, 4-phenyl-

Other names: Pyrazole, 4-phenyl-
4-(C6H5)-pyrazole
Inchi: InChI=1S/C9H8N2/c1-2-4-8(5-3-1)9-6-10-11-7-9/h1-7H,(H,10,11)
InchiKey: GPGKNEKFDGOXPO-UHFFFAOYSA-N
Formula: C9H8N2
SMILES: c1ccc(-c2cn[nH]c2)cc1
Mol. weight [g/mol]: 144.17
CAS: 10199-68-5

Physical Properties

Property code	Value	Unit	Source
affp	906.00	kJ/mol	NIST Webbook
basg	871.80	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=C10199685&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