

1H-Imidazole, 2-phenyl-

Other names:	2-phenyl-1H-imidazole 2-phenylimidazole imidazole, 2-phenyl-
Inchi:	InChI=1S/C9H8N2/c1-2-4-8(5-3-1)9-10-6-7-11-9/h1-7H,(H,10,11)
InchiKey:	ZCUJYXPAKHMBAZ-UHFFFAOYSA-N
Formula:	C9H8N2
SMILES:	c1ccc(-c2ncc[nH]2)cc1
Mol. weight [g/mol]:	144.17
CAS:	670-96-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	1.595		Crippen Method
mcvol	114.410	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	17.81	kJ/mol	420.00	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of Imidazoles, Benzimidazoles, and Phenylimidazoles	https://www.doi.org/10.1021/je049907t
McGowan Method	http://link.springer.com/article/10.1007/BF02311772
McGowan Method, 1-Chlorobutane, Toluene, and 2-Nitrotoluene:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C670962&Units=SI
NIST Webbook:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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