

2-PHENYLIMIDAZOLE

Other names:	2-phenyl-1H-imidazole 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]:	144.18

Physical Properties

Property code	Value	Unit	Source
hf	244.30	kJ/mol	Cheméo Relay (1.0)
logp	1.595		Crippen Method
mccvol	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Solubility of Imidazoles, Benzimidazoles, and Phenylimidazoles in Dichloromethane, 1-Chlorobutane, Toluene, and 2-Nitrotoluene:	https://www.doi.org/10.1021/je049907t http://webbook.nist.gov/cgi/cbook.cgi?ID=C670962&Units=SI

Legend

hf:	Enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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