

1H-Imidazole, 4,5-diphenyl-

Other names:	4,5-Diphenylglyoxaline 4,5-Diphenylimidazole 4,5-diphenyl-1H-imidazole 4.5-Diphenylimidazole Imidazole, 4,5-diphenyl-
Inchi:	InChI=1S/C15H12N2/c1-3-7-12(8-4-1)14-15(17-11-16-14)13-9-5-2-6-10-13/h1-11H,(H,16
InchiKey:	CPHGOBGXZQKCKI-UHFFFAOYSA-N
Formula:	C15H12N2
SMILES:	c1ccc(-c2nc[nH]c2-c2ccccc2)cc1
Mol. weight [g/mol]:	220.27
CAS:	668-94-0

Physical Properties

Property code	Value	Unit	Source
hfus	34.19	kJ/mol	Solubility of Imidazoles, Benzimidazoles, and Phenylimidazoles in Dichloromethane, 1-Chlorobutane, Toluene, and 2-Nitrotoluene
log10ws	-5.66		Crippen Method
logp	3.262		Crippen Method
mcvol	175.190	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	32.34	kJ/mol	505.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C668940&Units=SI

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
Solubility of Imidazoles, Benzimidazoles, and Phenylimidazoles in Dichloromethane, 1-Chlorobutane, Toluene, and 2-Nitrotoluene: <https://www.doi.org/10.1021/je049907t>

Legend

hfus: Enthalpy of fusion at standard conditions
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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