

1H-Benzimidazole, 2-methyl-

Other names:	1H-2-Methylbenzimidazol 1H-2-Methylbenzimidazole 2-Methyl-1H-benzimidazole 2-Methylbenzimidazole Acetamidine, N-N'-o-phenylene- Benzimidazole, 2-methyl- Methyl-2-benzimidazole
Inchi:	InChI=1S/C8H8N2/c1-6-9-7-4-2-3-5-8(7)10-6/h2-5H,1H3,(H,9,10)
InchiKey:	LDZYRENCLPUXAX-UHFFFAOYSA-N
Formula:	C8H8N2
SMILES:	Cc1nc2ccccc2[nH]1
Mol. weight [g/mol]:	132.16
CAS:	615-15-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Aqueous Solubility Prediction Method
logp	1.389		Crippen Method
mcvol	104.620	ml/mol	McGowan Method
tf	449.48	K	Aqueous Solubility Prediction Method
tf	451.43	K	Solubility of Benzimidazoles in Alcohols
tf	451.43	K	Solubility of Imidazoles, Benzimidazoles, and Phenylimidazoles in Dichloromethane, 1-Chlorobutane, Toluene, and 2-Nitrotoluene

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.49	kJ/mol	451.40	NIST Webbook

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C615156&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Solubility of Benzimidazoles in Alcohols: <https://www.doi.org/10.1021/je020228x>

Solubility of Imidazoles, Benzimidazoles, and Phenylimidazoles <https://www.doi.org/10.1021/je049907t>

in Dichloromethane, 1-Chlorobutane, Toluene, and 2-Nitrotoluene:

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

tf: Normal melting (fusion) point

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