

WIKIPEDIA

Benzimidazole

Benzimidazole is a heterocyclic aromatic organic compound. This bicyclic compound may be viewed as fused rings of the aromatic compounds benzene and imidazole. It is a colorless solid.

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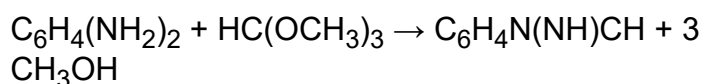
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Preparation

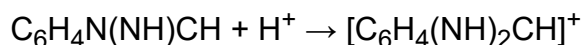
Benzimidazole is produced by condensation of o-phenylenediamine with formic acid,^[2] or the equivalent trimethyl orthoformate:



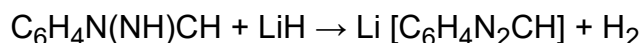
2-substituted derivatives are obtained when the condensation is conducted with aldehydes in place of formic acid, followed by oxidation.^[3]

Reactions

Benzimidazole is a base:

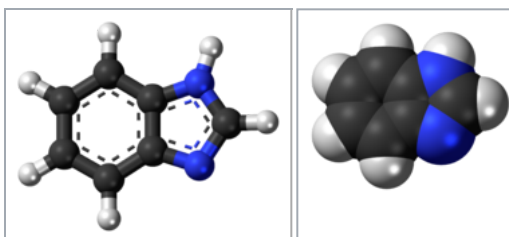
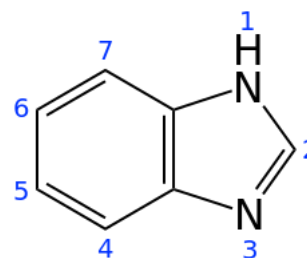


It can also be deprotonated with stronger bases:



The imine can be alkylated and also serves as a ligand in coordination chemistry. The most prominent benzimidazole complex features *N*-ribosyl-dimethylbenzimidazole as found

Benzimidazole



Names

Preferred IUPAC name

1*H*-1,3-Benzimidazole

Other names

1*H*-Benzo[*d*]imidazole

Identifiers

CAS Number

51-17-2 (https://commonchemistry.cas.org/detail?cas_rn=51-17-2) ✓

3D model (JSmol)

Interactive image (<https://chemapps.stolaf.edu/jmol/jmol.php?model=c1ccc2c%28c1%29%5BnH%5Dcn2>)

Beilstein Reference

109682

ChEBI

CHEBI:41275 (<https://www.ebi.ac.uk/chebi/searchId.do?chebiId=41275>) ✓

ChEMBL

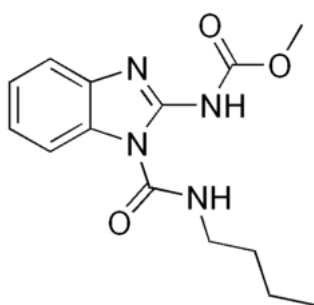
ChEMBL306226 (<https://www.ebi.ac.uk/chembl/db/index.php/compound>)

in vitamin B₁₂.^[4]

N,N'-Dialkylbenzimidazolium salts are precursors to certain *N*-heterocyclic carbenes.^{[5][6]}

Applications

Benzimidazoles are often bioactive. Many anthelmintic drugs (albendazole, mebendazole, triclabendazole etc.) belong to the benzimidazole class of compounds. Benzimidazole fungicides are commercialized. They act by binding to the fungal microtubules and stopping hyphal growth. It also binds to the spindle microtubules and blocks nuclear division.



Benomyl (Benlate) is a fungicide with a benzimidazole core

The proton-pump inhibitors (antacids) omeprazole, lansoprazole, pantoprazole, rabeprazole, and tenatoprazole all contain a benzimidazole group. Other pharmaceutical drugs which contain a benzimidazole group include galeterone, mavatrep, and dovitinib, as well as the benzimidazole opioids such as etonitazene. Benzimidazole derivatives are among the top frequently used ring systems for small molecule drugs listed by the US FDA.^[7]

In printed circuit board manufacturing, benzimidazole can be used as an organic solderability preservative.

Several dyes are derived from benzimidazoles.^[8]

See also


- Benzimidazoline
- Polybenzimidazole, a high performance fiber

References

- Walba, H. & Isensee, R. W. Acidity constants of some arylimidazoles and their cations. J. Org. Chem. 26, 2789-2791 (1961).

	d/inspect/ChEMBL306226) [✓]
ChemSpider	5593 (https://www.chemspider.com/Chemical-Structure.5593.html) [✓]
DrugBank	DB02962 (https://www.drugbank.ca/drugs/DB02962)
ECHA InfoCard	100.000.075 (https://echa.europa.eu/substance-information/-/substance-information/100.000.075)
EC Number	200-081-4
Gmelin Reference	3106
KEGG	C02009 (https://www.kegg.jp/entry/C02009) [✓]
PubChem CID	5798 (https://pubchem.ncbi.nlm.nih.gov/compound/5798)
UNII	E24GX49LD8 (https://fdasis.nlm.nih.gov/srs/srsdirect.jsp?regno=E24GX49LD8) [✓]
CompTox Dashboard (EPA)	DTXSID8024573 (https://comptox.epa.gov/dashboard/chemical/details/DTXSID8024573)
InChI	InChI=1S/C7H6N2/c1-2-4-7-6(3-1)8-5-9-7/h1-5H,(H,8,9) [✓] Key: HYZJCKYKOHLVJF-UHFFFAOYSA-N [✓]
	InChI=1/C7H6N2/c1-2-4-7-6(3-1)8-5-9-7/h1-5H,(H,8,9) Key: HYZJCKYKOHLVJF-UHFFFAOYAX
SMILES	c1ccc2c(c1)[nH]cn2
Properties	
Chemical formula	C ₇ H ₆ N ₂
Molar mass	118.139 g·mol ⁻¹

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- H. A. Barker; R. D. Smyth; H. Weissbach; J. I. Toohey; J. N. Ladd & B. E. Volcani (February 1, 1960). "Isolation and Properties of Crystalline Cobamide Coenzymes Containing Benzimidazole or 5,6-Dimethylbenzimidazole" (<https://doi.org/10.1016%2FS0021-9258%2818%2969550-X>). *Journal of Biological Chemistry*. **235** (2): 480–488. doi:10.1016/S0021-9258(18)69550-X (<https://doi.org/10.1016%2FS0021-9258%2818%2969550-X>). PMID 13796809 (<https://pubmed.ncbi.nlm.nih.gov/13796809>).
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- H. V. Huynh; J. H. H. Ho; T. C. Neo; L. L. Koh (2005). "Solvent-controlled selective synthesis of a trans-configured benzimidazolone-2-ylidene palladium(II) complex and investigations of its Heck-type catalytic activity". *Journal of Organometallic Chemistry*. **690** (16): 3854–3860. doi:10.1016/j.jorganchem.2005.04.053 (<http://doi.org/10.1016%2Fj.jorganchem.2005.04.053>).
- Taylor, R. D.; MacCoss, M.; Lawson, A. D. G. *J Med Chem* 2014, 57, 5845.>
- Horst Berneth "Methine Dyes and Pigments" in *Ullmann's Encyclopedia of Industrial Chemistry*, 2008, Wiley-VCH, Weinheim. doi:10.1002/14356007.a16_487.pub2 (https://doi.org/10.1002%2F14356007.a16_487.pub2)

Melting point	170 to 172 °C (338 to 342 °F; 443 to 445 K)
Acidity (pK _a)	12.8 (for benzimidazole) and 5.6 (for the conjugate acid) ^[1]
Hazards	
GHS labelling:	
Pictograms	
Signal word	Warning
Hazard statements	H302, H315, H319, H335
Precautionary statements	P261, P264, P270, P271, P280, P301+P312, P302+P352, P304+P340, P305+P351+P338, P312, P321, P330, P332+P313, P337+P313, P362, P403+P233, P405, P501
Safety data sheet (SDS)	External MSDS (http://msds.chem.ox.ac.uk/BE/benzimidazole.html)
<p>Except where otherwise noted, data are given for materials in their standard state (at 25 °C [77 °F], 100 kPa).</p> <p>✓ verify (what is ✗ ?)</p> <p>Infobox references</p>	

Further reading

- Grimmett, M. R. (1997). *Imidazole and benzimidazole synthesis*. Boston: Academic Press. ISBN 0-12-303190-7.

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