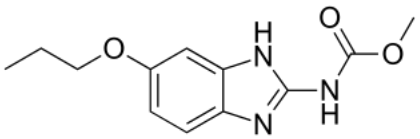
WIKIPEDIA

Oxibendazole

Oxibendazole is a benzimidazole drug that is used to protect against roundworms, strongyles, threadworms, pinworms and lungworm infestations in horses and some domestic pets.[1][2] It is usually white to yellowish in appearance, and may take the form of a powder, tablet or paste.

Synthesis

Oxibendazole

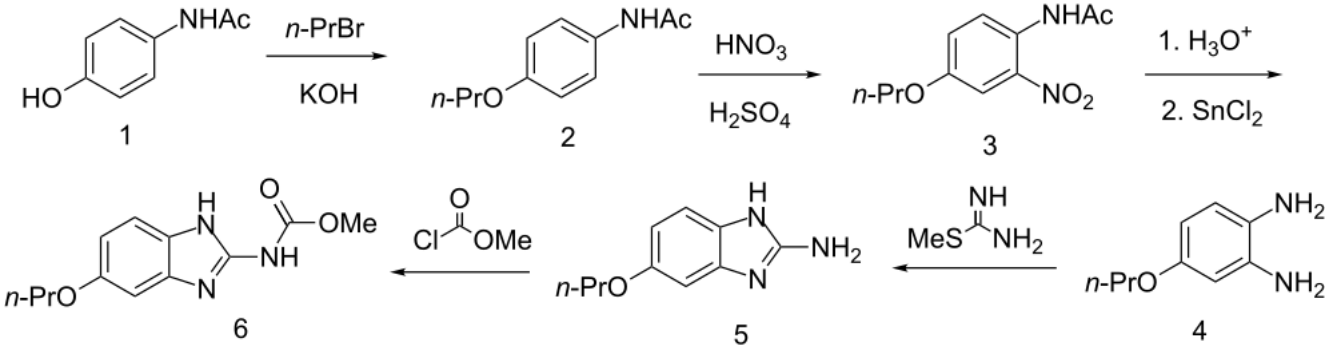


Clinical data	
AHFS/Drugs.com	International Drug Names (https://www.drugs.com/international/oxibendazole.html)
ATCvet code	QP52AC07 (WHO (https://www.whocc.no/atcvet/atcvet_index/?code=QP52AC07))
Legal status	
Legal status	Veterinary use only
Identifiers	
IUPAC name	Methyl *N*-(6-propoxy-1*H*-benzimidazol-2-yl)carbamate
CAS Number	20559-55-1 (https://commonchemistry.cas.org/detail?cas_rn=20559-55-1) ✓
PubChem CID	4622 (https://pubchem.ncbi.nlm.nih.gov/compound/4622)
ChemSpider	4461 (https://www.chemspider.com/Chemical-Stru

	cture.4461.html) ✗
UNII	022N12KJ0X (https://precision.fda.gov/uniisearch/srs/unii/022N12KJ0X)
KEGG	D05293 (https://www.kegg.jp/entry/D05293) ✓
CompTox Dashboard (EPA)	DTXSID5045625 (https://comptox.epa.gov/dashboard/chemical/details/DTXSID5045625)
ECHA InfoCard	100.039.873 (https://echa.europa.eu/substance-information/-/substanceinfo/100.039.873)
Chemical and physical data	
Formula	$C_{12}H_{15}N_3O_3$
Molar mass	249.270 g·mol^{-1}
3D model (JSmol)	Interactive image (https://chemapps.stolaf.edu/jmol/jmol.php?model=CCCOC1%3DCC2%3DC%28C%3DC1%29N%3DC%28N2%29NC%28%3DO%29OC)
SMILES	CCCOC1=CC2=C(C=C1)N=C(N2)NC(=O)OC
InChI	InChI=1S/C12H15N3O3/c1-3-6-18-8-4-5-9-10(7-8)14-11(13-9)15-12(16)17-2/h4-5,7H,3,6H2,1-2H3,(H2,13,14,15,16) ✗

Key:RAOCRURYZCVHMG-UHFFFAOYSA-N ✗

✗✓ (what is this?) (verify)



Oxibendazole synthesis:[3]

4-Hydroxyacetamide (**1**) is alkylated with *n*-propyl bromide in the presence of potassium hydroxide to give the ether (**2**). Nitration of this product with nitric and sulfuric acids proceeds at the position *ortho* to the amide group (**3**), which is then reduced with $SnCl_2$ to yield the phenylenediamine derivative (**4**). Reaction of that intermediate with *S*-methyl isothiourea proceeds first by aromatic cyclisation to the guanidine derivative followed by elimination of methyl mercaptan to yield the 2-aminobenzimidazole system (**5**). Acylation with methyl chloroformate results in the formation of a urethane on the amino group to produce oxibendazole (**6**).

References

1. Theodorides VJ, Chang J, DiCuollo CJ, Grass GM, Parish RC, Scott GC (December 1973). "Oxibendazole, a new broad spectrum anthelmintic effective against gastrointestinal nematodes of domestic animals". *The British Veterinary Journal*. **129** (6): xcontdvii–scvi. doi:10.1016/s0007-1935(17)36351-0 (https://doi.org/10.1016%2Fs0007-1935%2817%2936351-0). PMID 4779247 (https://pubmed.ncbi.nlm.nih.gov/4779247).
2. Bowman DD (2009). "Chapter 6: Anti-parasitic Drugs" (https://books.google.com/books?id=g_tBWVBevM0C&pg=PA280). *Georgis' parasitology for veterinarians* (9th ed.). St. Louis, Mo.: Saunders/Elsevier. p. 280. ISBN 978-1-4160-4412-3.
3. GB 1123317 (https://worldwide.espacenet.com/textdoc?DB=EPODOC&IDX=GB1123317), "Anthelmintic compositions containing benzimidazole derivatives", published 1968-08-14, assigned to Smith Kline French Labs; US 3574845 (https://worldwide.espacenet.com/textdoc?DB=EPODOC&IDX=US3574845), Actor PP, Pagano JF, "Anthelmintic compositions and methods employing esters of benzimidazolyl carbamic acids and their thio analogs", issued 13 April 1971, assigned to Smith Kline and French Laboratories Ltd