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Bamnidazole

Cat. No.: B1329383

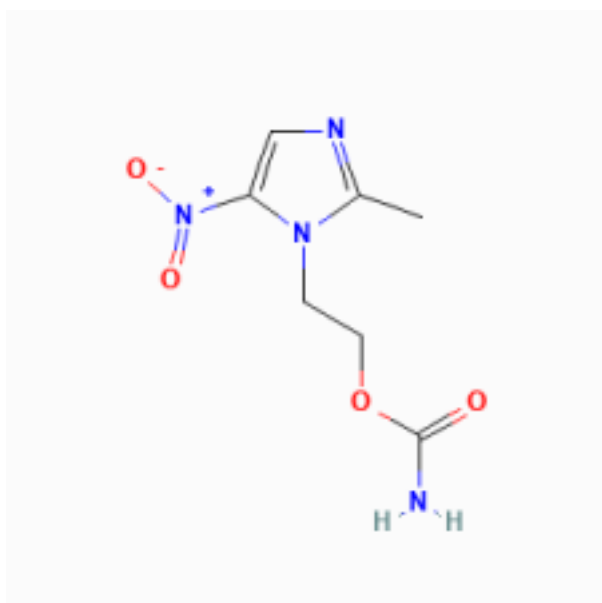
CAS No.: 31478-45-2

M. Wt: 214.18 g/mol

InChI JOVXEDBYAWFQXX-UHFFFAOYSA-N

Key:

Attention:For research use only. Not for human or veterinary use.



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Overview

1. Description
2. Mechanism of action
3. Properties
4. Retrosynthesis analysis
5. Disclaimer

Description

Bamnidazole is a useful research compound. Its molecular formula is C₇H₁₀N₄O₄ and its molecular weight is 214.18 g/mol. The purity is usually 95%.

The exact mass of the compound this compound is unknown and the complexity rating of the compound is unknown. The compound has been submitted to the National Cancer Institute (NCI)

for testing and evaluation and the Cancer Chemotherapy National Service Center (NSC) number is 329676. The storage condition is unknown. Please store according to label instructions upon receipt of goods.

BenchChem offers high-quality this compound suitable for many research applications. Different packaging options are available to accommodate customers' requirements. Please inquire for more information about this compound including the price, delivery time, and more detailed information at info@benchchem.com.

Mechanism of Action

Target of Action

- **Primary Targets** : Benznidazole primarily targets *Trypanosoma cruzi*, the causative organism of Chagas disease (<https://go.drugbank.com/drugs/DB11989>) [”] (<https://go.drugbank.com/drugs/DB11989>).

Mode of Action

- **Mechanism** : It generates radical species that can damage the parasite's DNA or cellular machinery (<https://go.drugbank.com/drugs/DB11989>) [”] (<https://en.wikipedia.org/wiki/Benznidazole>).
- These radical metabolites likely bind to proteins, lipids, DNA, and RNA, causing damage to these macromolecules (<https://go.drugbank.com/drugs/DB11989>) [”] (<https://go.drugbank.com/drugs/DB11989>).
- Increased trypanosomal death may occur due to inflammation caused by macromolecule damage and elevated interferon- γ levels (<https://go.drugbank.com/drugs/DB11989>) [”] (<https://go.drugbank.com/drugs/DB11989>).

Biochemical Pathways

- **Downstream Effects** : DNA undergoes extensive unpacking, with overexpression of DNA repair proteins (<https://go.drugbank.com/drugs/DB11989>) [”] (<https://go.drugbank.com/drugs/DB11989>).

Pharmacokinetics

- **Absorption** : Benznidazole is rapidly absorbed after oral administration (<https://go.drugbank.com/drugs/DB11989>) [”] (<https://www.medicines.com/drug/benznidazole/hcp>).
- **Bioavailability** : It has a high bioavailability of 91.7% (<https://go.drugbank.com/drugs/DB11989>) [”] (<https://go.drugbank.com/drugs/DB11989>).
- **Distribution** : The apparent volume of distribution is 39.19 L (<https://go.drugbank.com/drugs/DB11989>) [”] (<https://go.drugbank.com/drugs/DB11989>).
- **Metabolism** : Nitro reduction by *Trypanosoma cruzi* nitroreductases and cytochrome P450 enzymes (<https://go.drugbank.com/drugs/DB11989>) [”] (<https://go.drugbank.com/drugs/DB11989>).

/DB11989).

- **Excretion** : Primarily via urine (68%) and feces (21%) (<https://go.drugbank.com/drugs/DB11989>) [”](https://go.drugbank.com/drugs/DB11989) (<https://go.drugbank.com/drugs/DB11989>).
- **Time to Peak** : Median time to peak concentration is 2 hours (<https://go.drugbank.com/drugs/DB11989>) [”](https://www.medicines.com/drug/benznidazole/hcp) (<https://www.medicines.com/drug/benznidazole/hcp>).

Properties

IUPAC Name	2-(2-methyl-5-nitroimidazol-1-yl)ethyl carbamate	Source
InChI	InChI=1S/C7H10N4O4 /c1-5-9-4-6(11(13)14)10(5)2-3-15-7(8)12 /h4H,2-3H2,1H3,(H2,8,12)	Source
InChI Key	JOVXEDBYAWFQQX-UHFFFAOYSA-N	Source
Canonical SMILES	<chem>CC1=NC=C(N1CCOC(=O)N)[N+](=O)[O-]</chem>	Source
Molecular Formula	C7H10N4O4	Source
DSSTOX Substance ID	DTXSID70185378	Source
Molecular Weight	214.18 g/mol	Source
CAS No.	31478-45-2	Source

Retrosynthesis Analysis

AI-Powered Synthesis Planning: Our tool employs the Template_relevance Pistachio, Template_relevance Bkms_metabolic, Template_relevance Pistachio_ringbreaker, Template_relevance Reaxys, Template_relevance Reaxys_biocatalysis model, leveraging a vast database of chemical reactions to predict feasible synthetic routes.

One-Step Synthesis Focus: Specifically designed for one-step synthesis, it provides concise and direct routes for your target compounds, streamlining the synthesis process.

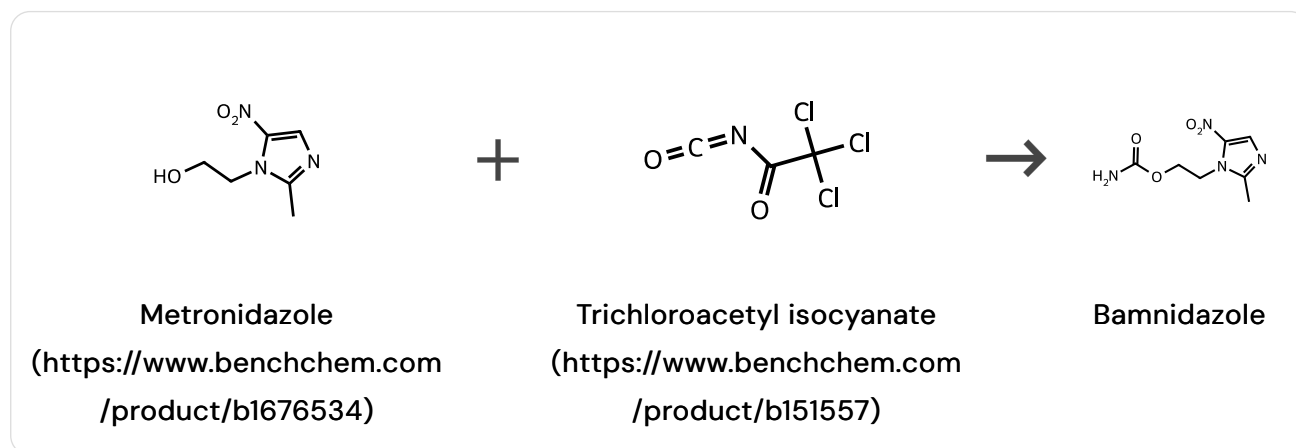
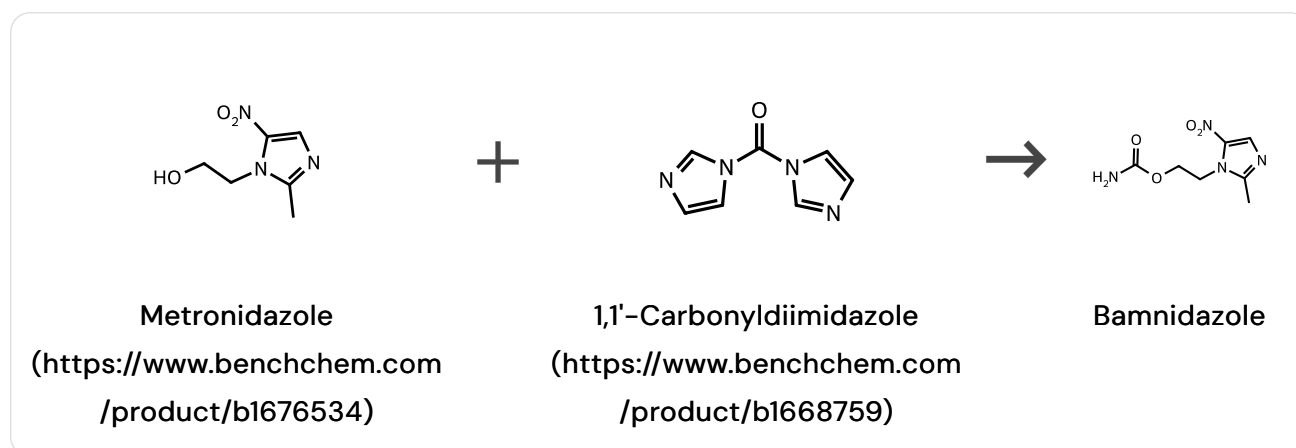
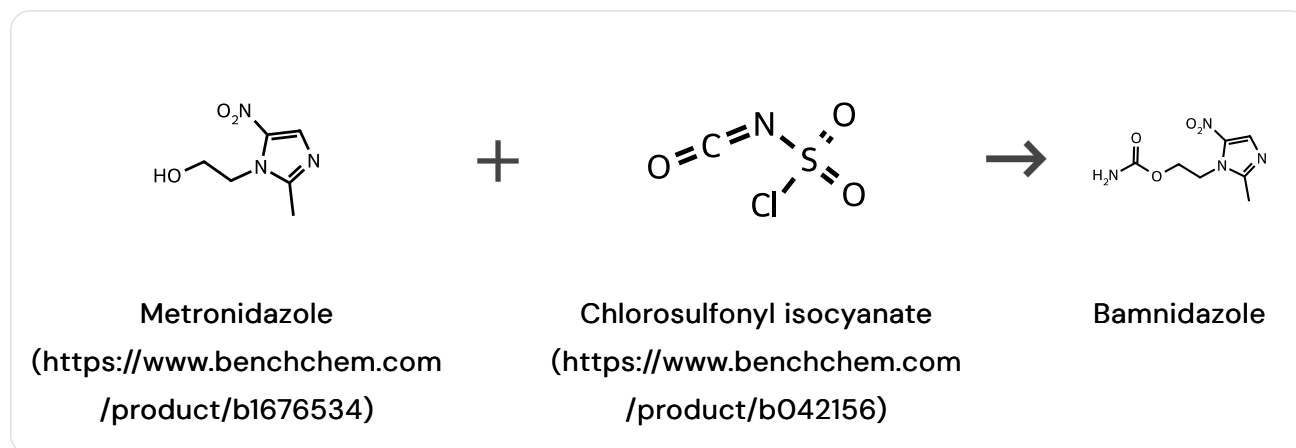
Accurate Predictions: Utilizing the extensive PISTACHIO, BKMS_METABOLIC, PISTACHIO_RINGBREAKER, REAXYS, REAXYS_BIOCATALYSIS database, our tool offers high-accuracy predictions, reflecting the latest in chemical research and data.

Strategy Settings

Precursor scoring Relevance Heuristic

Min. plausibility	0.01
Model	Template_relevance
Template Set	Pistachio/Bkms_metabolic/Pistachio_ringbreaker/Reaxys /Reaxys_biocatalysis
Top-N result to add to graph	6

Feasible Synthetic Routes



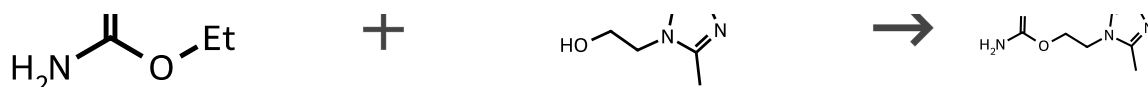
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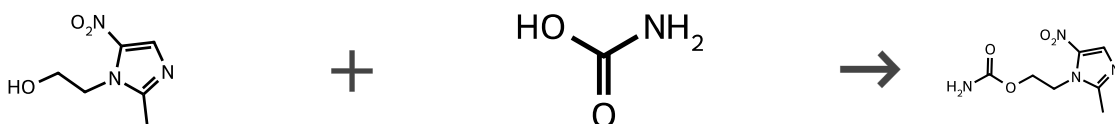




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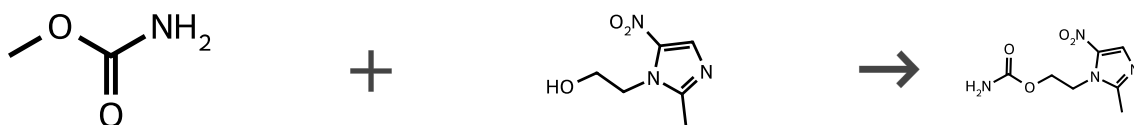
Bamnidazole



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Carbamic acid
 (<https://www.benchchem.com/product/b1208785>)

Bamnidazole



Methyl carbamate
 (<https://www.benchchem.com/product/b145844>)

Metronidazole
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Bamnidazole

More For Retrosynthesis Analysis

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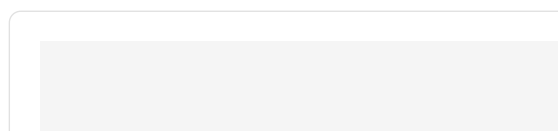
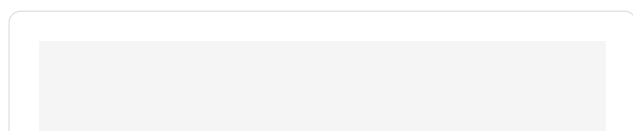
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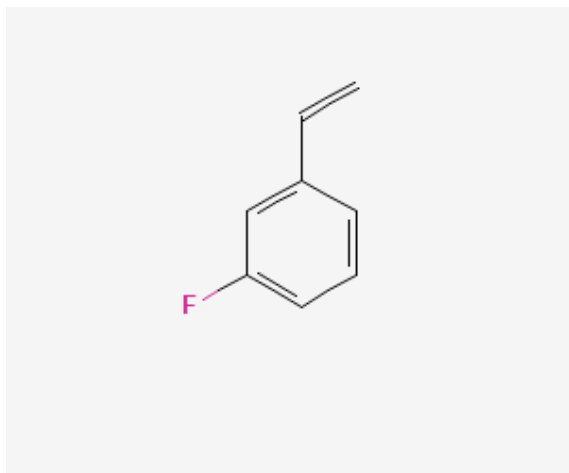
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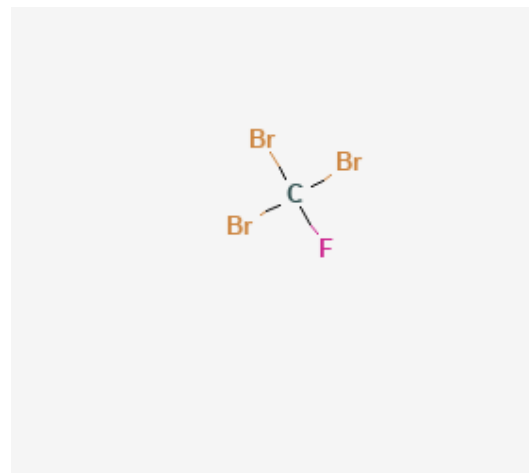
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