

LLM output:

```
### Step 1: Check mismatch between derived SMILES and target
- **Target molecule**: `CN(C)CCO`
- **Derived molecule from original reasoning**: `N(CC)(CCO)`
```

Now compare:

```
- `N(CC)(CCO)` describes a nitrogen with **two -CH2CH3 substituents** (ethyl groups) and one hydroxyethyl group, i.e., a trialkylamine.
- The target `CN(C)CCO` clearly shows: nitrogen with **two methyl groups** (`CN(C)`) and one -CH2CH2OH group.
- Therefore, the CoT erroneously attached **ethyl groups** instead of **methyl groups**.
```

```
### Step 2: Identify the mistake in reasoning
```

```
- The error is in step 4 of the reasoning:
```

```
> "With two methyl groups attached to the nitrogen, the amine becomes N(CH3)2, while the hydroxyl group remains. The complete SMILES is N(CC)(CCO)."

```

Current Record: 320 / 332

smile:

CN(C)CCO

explain:

The molecule is a tertiary amine that is ethanolamine having two N-methyl substituents. It has a role as a curing agent and a radical scavenger. It is a tertiary amine and a member of ethanolamines.

cot:

<Thinking>

To derive the SMILES representation for the described molecule, let's break down the components step by step.

1. **Identify the Base Structure**: The base structure is ethanolamine, which has the formula H2N-CH2-CH2-OH. In SMILES, this is represented as `NCCO`.

2. **Identify the Substituents**: The description states that there are two N-methyl substituents. This means that both methyl groups (-CH3) are attached to the nitrogen atom.

3. **Construct the New Structure**: With two methyl groups attached to the nitrogen, the amine becomes N(CH3)2, while the hydroxyl group remains on the terminal carbon.

4. **Final Structure Representation**: The complete SMILES for this substituted ethanolamine is **N(CC)(CCO)**.

score:

2

reason:

smile [curated]:

CN(C)CCO

explain [curated]:

The molecule is a tertiary amine that is ethanolamine having two N-methyl substituents. It has a role as a curing agent and a radical scavenger. It is a tertiary amine and a member of ethanolamines.

cot [curated]:

<Thinking>

To derive the SMILES representation for the described molecule, let's break down the components step by step.

1. **Identify the Base Structure**: The base structure is ethanolamine, which has the formula H2N-CH2-CH2-OH. In SMILES, this is represented as `NCCO`.

2. **Identify the Substituents**: The description states that there are two N-methyl substituents. This means that both methyl groups (-CH3) are attached to the nitrogen atom.

3. **Construct the New Structure**: With two methyl groups attached to the nitrogen, the amine becomes N(CH3)2, while the hydroxyl group remains on the terminal carbon.

4. **Final Structure Representation**: The complete SMILES for this

score [curated]:

3

reason [curated]:

Previous

Next

Save Changes

Export Records

Jump to:

320

Jump

 View Modified

 Export Modified

LLM assistant