



# Green Chemistry Simulation Report

## Test Reaction

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### Product Information

#### Test Product

**Molecular Weight:** 100 g/mol

**Actual Mass:** 10 g

**Carbon Atoms:** N/A

### Key Green Chemistry Metrics

ATOM ECONOMY

**80.0%**

PMI

**12.0**

E-FACTOR

**N/A**

RME

**N/A%**

CARBON EFF.

**N/A%**

STOICH. FACTOR

**N/A**

WATER  
INTENSITY

**N/A**

ENERGY

**N/A**

SOLVENT INT.

**N/A**

CARBON  
FOOTPRINT

**N/A**

#### Metrics Interpretation Guide:

- Atom Economy (AE):**  $\geq 80\%$  excellent, 60-80% good,  $< 60\%$  needs improvement
- PMI:**  $< 10$  pharmaceutical,  $< 5$  fine chemicals,  $< 1$  ideal
- E-Factor:** Lower is better;  $< 1$  pharmaceutical,  $< 5$  fine chemicals
- RME:**  $\geq 80\%$  excellent, 60-80% good,  $< 60\%$  needs improvement
- Carbon Efficiency (CE):**  $\geq 80\%$  excellent, 60-80% good,  $< 60\%$  needs improvement

## Reactants

#	Name	MW (g/mol)	Mass (g)	C Atoms	Eq. Used
1	Reactant 1	80	8	N/A	N/A

## Solvents

#	Name	Mass (g)	Recovery
No solvents			

## Mass Balance Breakdown

Reactant Mass	0 g
Catalyst Mass	0 g
Total Solvent Mass	0 g
Aqueous Washes	0 g
Auxiliaries (Drying)	0 g
Total Input Mass	0 g
Product Mass	0 g

## AI-Powered Recommendations

- No suggestions available. Run simulation to generate insights.