



Green Chemistry Simulation Report

Test PDF Generation

Generated: October 04, 2025 at 01:37 PM

Product Information

Test Product

Molecular Weight: 180.0 g/mol

Actual Mass: 10.0 g

Carbon Atoms: None

Key Green Chemistry Metrics

ATOM ECONOMY

85.5%

PMI

2.5

E-FACTOR

1.5

RME

75.0%

CARBON EFF.

80.0%

STOICH. FACTOR

3.5

WATER
INTENSITY

10.0

ENERGY

2.0

SOLVENT INT.

N/A

CARBON
FOOTPRINT

1000.0

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 A	100.0	15.0	None	None

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.