



Green Chemistry Simulation Report

Async Verification Test

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Product Information

Test Product

Molecular Weight: 100 g/mol

Actual Mass: 10 g

Carbon Atoms: 5

Key Green Chemistry Metrics

ATOM ECONOMY

85.0%

PMI

15.0

E-FACTOR

14.0

RME

50.0%

CARBON EFF.

80.0%

STOICH. FACTOR

N/A

WATER
INTENSITY

N/A

ENERGY

N/A

SOLVENT INT.

5.0

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	Test Reactant	80	8	4	1.0

Solvents

#	Name	Mass (g)	Recovery
1	Water	50	0%

Mass Balance Breakdown

Reactant Mass	8.0 g
Catalyst Mass	0 g
Total Solvent Mass	50.0 g
Aqueous Washes	0 g
Auxiliaries (Drying)	0 g
Total Input Mass	0 g
Product Mass	10.0 g

AI-Powered Recommendations

- No suggestions available. Run simulation to generate insights.