



Green Chemistry Simulation Report

Test from FastAPI

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Product Information

Test Product

Molecular Weight: 180.16 g/mol

Actual Mass: 10.0 g

Carbon Atoms: 9

Key Green Chemistry Metrics

ATOM ECONOMY

85.5%

PMI

15.88

E-FACTOR

14.88

RME

48.78%

CARBON EFF.

82.14%

STOICH. FACTOR

1.1

WATER
INTENSITY

None

ENERGY

None

SOLVENT INT.

0.0

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	138.12	8.3	7	1.0

Solvents

#	Name	Mass (g)	Recovery
No solvents			

Mass Balance Breakdown

Reactant Mass	8.3 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	10.0 g

AI-Powered Recommendations

- No suggestions available. Run simulation to generate insights.