



Green Chemistry Simulation Report

Synthesis of Aspirin

Generated: October 03, 2025 at 11:57 PM

Product Information

aspirin

Molecular Weight: 180.16 g/mol

Actual Mass: 10.0 g

Carbon Atoms: 9

Key Green Chemistry Metrics

ATOM ECONOMY

75.0%

PMI

31.56

E-FACTOR

30.56

RME

48.78%

CARBON EFF.

55.59%

STOICH. FACTOR

1.1

WATER
INTENSITY

25.0

ENERGY

0.0525

SOLVENT INT.

19.51

CARBON
FOOTPRINT

26.25

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	salicylic acid	138.12	8.3	7	1.0
2	acetic anhydride	102.09	12.2	4	1.2

Solvents

#	Name	Mass (g)	Recovery
1	ethyl acetate	45.1	60.0%
2	water	150.0	0.0%

Mass Balance Breakdown

Reactant Mass	20.5 g
Catalyst Mass	0 g
Total Solvent Mass	195.1 g
Aqueous Washes	100 g
Auxiliaries (Drying)	0 g
Total Input Mass	315.6 g
Product Mass	10 g

AI-Powered Recommendations

- No suggestions available. Run simulation to generate insights.

