Green Chemistry Simulation Report

Synthesis of Aspirin

Generated: October 03, 2025 at 11:14 PM

Product Information

aspirin

Molecular Weight: 180.16 g/mol

Actual Mass: 10.0 g

Carbon Atoms: 9

Key Green Chemistry Metrics

ATOM ECONOMY	PMI	E-FACTOR	RME	CARBON EFF.
75.0%	31.56	30.56	48.78%	55.59%

STOICH. FACTOR	WATER INTENSITY	ENERGY	SOLVENT INT.	CARBON FOOTPRINT
1.1	25.0	0.0525	19.51	26.25

Metrics Interpretation Guide:

- **Atom Economy (AE):** ≥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:** ≥80% excellent, 60-80% good, <60% needs improvement
- **Carbon Efficiency (CE):** ≥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.