



Green Chemistry Simulation Report

Synthesis of Aspirin

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Product Information

Aspirin

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

10.0

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%
2	Water	150.0	0%

Catalysts

#	Name	MW (g/mol)	Mass (g)
1	Sulfuric Acid	98.08	0.5

Mass Balance Breakdown

Reactant Mass	20.5 g
Catalyst Mass	0.5 g
Total Solvent Mass	195.1 g
Aqueous Washes	100.0 g
Auxiliaries (Drying)	0.0 g
Total Input Mass	316.1 g
Product Mass	10.0 g

AI-Powered Recommendations

- Consider replacing acetic anhydride with a greener acylating agent
- Explore water-based solvent systems to reduce organic solvent use
- Optimize catalyst loading - sulfuric acid can be reduced
- Implement solvent recovery to improve sustainability metrics

Green Toolkit - Sustainable Chemistry Analysis Platform

This report was automatically generated. All metrics calculated according to standard green chemistry principles.

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