Safety Data Sheet (SDS)

Generated from SMILES using AI & Cheminformatics

Compound: 4-(4-hydroxy-3-methoxyphenyl)butan-2-one | Generated on: 2025-08-04 15:15

1. Chemical Product and Company Identification

Product Identifier	4-(4-hydroxy-3-methoxyphenyl)butan-2-one
Company	Automated SDS Generator
Address	N/A
Emergency Phone	N/A
Recommended Use	Research Use Only

2. Composition and Information on Ingredients

Name	4-(4-hydroxy-3-methoxyphenyl)butan-2-one	
CAS Number	Not available	
Molecular Formula	C11H14O3	
Purity/Concentration	100% (pure compound)	

3. Hazards Identification

Signal Word	Warning
GHS Pictograms	Not classified
Hazard Statements	No significant hazards identified
Precautionary Statements	 P210: Keep away from heat, hot surfaces, sparks, open flames. P241: Use explosion-proof electrical/ventilation equipment. P261: Avoid breathing dust/fume/gas/mist/vapors/spray. P280: Wear protective gloves/protective clothing/eye protection/face protection. P305+P351+P338: IF IN EYES: Rinse cautiously with water for several minutes.
Physical Hazards	Not flammable
Health Hazards	None identified
Environmental Hazards	Low concern
Routes of Exposure	Inhalation, Skin Contact, Ingestion, Eye Contact
Acute and Chronic Effects	This substance is harmful if inhaled, swallowed, or absorbed through the skin. Chronic exposure may lead to liver, kidney, or respiratory damage.
Immediate Medical Attention	Seek medical attention immediately in case of exposure. Show SDS to physician.

4. First Aid Measures

Inhalation	Move to fresh air. If breathing is difficult, give oxygen.
Skin Contact	Flush with plenty of water. Remove contaminated clothing.
Eye Contact	Flush with water for at least 15 minutes.
Ingestion	Do NOT induce vomiting. Rinse mouth and consult a physician.

5. Fire and Explosion Data

Flash Point	Not flammable	
Flammable Limits	3.3% - 19% in air	
Extinguishing Media	Dry chemical, CO2, alcohol-resistant foam	
Special Hazards	Vapors may form explosive mixtures with air.	

6. Accidental Release Measures

Personal Precautions	Wear PPE, ensure ventilation	
Environmental Precautions	Prevent entry into drains or waterways	
Methods of Containment	Absorb with inert material (sand, vermiculite)	

7. Handling and Storage

Handling	Ground containers, use explosion-proof equipment
Storage	Store in a cool, well-ventilated place away from ignition sources

8. Exposure Controls/Personal Protection

TLV-TWA	100 ppm (300 mg/m³) for ethanol-like compounds	
Engineering Controls	Local exhaust ventilation	
Personal Protection	Safety goggles, gloves, lab coat	

9. Physical and Chemical Properties

Physical State	Liquid
Color	Colorless
Odor	Characteristic
Melting Point	Not available

Boiling Point	Not available
Solubility in Water	Highly soluble
Density	Approx. 0.79 g/cm³ (for alcohols)
Vapor Pressure	< 1 mmHg at 25°C
Molecular Weight	194.23 g/mol
LogP	1.92
Topological Polar Surface Area (TPSA)	46.53 Ų
Hydrogen Bond Donors	1
Hydrogen Bond Acceptors	3
Rotatable Bonds	4
Heavy Atom Count	14

10. Stability and Reactivity

Stability	Stable under normal conditions
Conditions to Avoid	Heat, flames, sparks
Incompatible Materials	Strong oxidizing agents
Hazardous Decomposition	Carbon monoxide, carbon dioxide

11. Toxicological Information

LD50 Oral Rat	5000 mg/kg
LC50 Inhalation Rat	Not available
Carcinogenicity	Not suspected
Mutagenicity	Negative
Toxicity Class	Class IV (Low)

12. Ecological Information

Ecotoxicity	Low concern
Biodegradability	Yes
Persistence	Low
Bioaccumulation	Low potential

13. Disposal Considerations

Disposal Method	Dispose in accordance with local regulations
Contaminated Packaging	Rinse and recycle or dispose properly

14. Transport Information

UN Number	UN1170
Proper Shipping Name	Ethanol or Ethyl Alcohol
Transport Hazard Class	3 (Flammable Liquid)
Packing Group	II

15. Other Regulatory Information

TSCA	Listed
DSL	Listed
WHMIS	Classified
GHS Regulation	GHS Rev 9 compliant

16. Other Information

Date Prepared	2025-08-04
Revision Number	1.0
Prepared By	Automated ADMET-SDS System
Disclaimer	Generated for research use only. Verify with lab testing.

Generated with ♥ for chemical safety

Disclaimer: This report is generated for research use only. Verify with lab testing and official sources before use.