

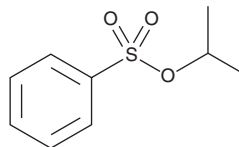
# PRODUCT INFORMATION



## Isopropyl Benzenesulfonate

Item No. 17795

**CAS Registry No.:** 6214-18-2  
**Formal Name:** benzenesulfonic acid, 1-methylethyl ester  
**Synonym:** Benzenesulfonic Acid isopropyl ester  
**MF:** C<sub>9</sub>H<sub>12</sub>O<sub>3</sub>S  
**FW:** 200.3  
**Purity:** ≥98%  
**UV/Vis.:** λ<sub>max</sub>: 217, 258, 264, 271 nm  
**Supplied as:** A neat oil  
**Storage:** -20°C  
**Stability:** ≥4 years



Information represents the product specifications. Batch specific analytical results are provided on each certificate of analysis.

### Laboratory Procedures

Isopropyl benzenesulfonate is supplied as a neat oil. A stock solution may be made by dissolving the isopropyl benzenesulfonate in the solvent of choice, which should be purged with an inert gas. Isopropyl benzenesulfonate is soluble in organic solvents such as ethanol, DMSO, and dimethyl formamide. The solubility of isopropyl benzenesulfonate in these solvents is approximately 30 mg/ml.

Isopropyl benzenesulfonate is sparingly soluble in aqueous buffers. For maximum solubility in aqueous buffers, isopropyl benzenesulfonate should first be dissolved in ethanol and then diluted with the aqueous buffer of choice. Isopropyl benzenesulfonate has a solubility of approximately 0.5 mg/ml in a 1:1 solution of ethanol:PBS (pH 7.2) using this method. We do not recommend storing the aqueous solution for more than one day.

### Description

Isopropyl benzenesulfonate is a sulfonate ester genotoxic impurity found in active pharmaceutical ingredients.<sup>1</sup> It has potential to exert toxic effects in bacterial and mammalian cells.

### Reference

1. Guo, T., Shi, Y., Zheng, L., *et al.* Rapid and simultaneous determination of sulfonate ester genotoxic impurities in drug substance by liquid chromatography coupled to tandem mass spectrometry: Comparison of different ionization modes. *J. Chromatogr. A* **1355**, 73-79 (2014).

**WARNING**  
THIS PRODUCT IS FOR RESEARCH ONLY - NOT FOR HUMAN OR VETERINARY DIAGNOSTIC OR THERAPEUTIC USE.

**SAFETY DATA**  
This material should be considered hazardous until further information becomes available. Do not ingest, inhale, get in eyes, on skin, or on clothing. Wash thoroughly after handling. Before use, the user must review the [complete](#) Safety Data Sheet, which has been sent via email to your institution.

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