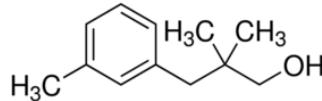


Certificate of Analysis

Product name: **β,β,3-Trimethylbenzenopropanol**
Product no.: **78329**
Reference Material
Lot no.: BCCC2880
Expiry Date: NOV 2023
Storage: -20°C ± 5°C; storage under Argon
Chemical formula: C₁₂H₁₈O
Molecular mass: 178.27 g/mol
CAS No. 103694-68-4
Metrological traceability (certified value): NIST SRM 84I (KHP)
Date of testing (certified value): 31 OCT 2019



Sample	Certified value ± Expanded uncertainty (<i>k</i> =2) Mass fraction (g/g) by quantitative NMR spectroscopy
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β,β,3-Trimethylbenzenopropanol **98.2 % ± 2.5 %**

Indicative values (not within scope of ISO/IEC 17025 accreditation)		
Test	Specification	Result
Appearance (Color)	Colorless or White	White
Appearance (Form)	Liquid or Solid	Solid
Purity (GC Area %)	≥ 98.0 %	99.5 %

Measurement method and uncertainty:

The certified value is assessed by quantitative NMR measurements (qNMR) within the scope of ISO/IEC 17025 accreditation. The uncertainty includes contributions from the primary reference material, the ambient conditions, weighing process, the measuring system, and any possible contributions from homogeneity and stability. It is calculated according to Eurachem/CITAC Guide "Quantifying uncertainty in analytical measurement" with a probability of 95%. The sole measurement uncertainty is calculated as

$$u_{\text{char}} = 1.5\% \text{ (g/g)} \text{ (*k*=2).}$$

Minimum sample size:

15 mg

Instructions for handling:

The Reference Material should be stored in the original bottle. Warm to room temperature before opening. After each use the bottle should be tightly closed and protected from excessive moisture and light.

Certificate issue date:

20 DEC 2019



ISO/IEC 17025
STS 0490

A. Rück

Dr. A. Rück – CRM Operations

J. Zell

Dr. P. Zell – Approving Officer



Further measurement information:

Please note that qNMR values can differ from chromatographic purity due to the presence of impurities/components (such as salts, water, residual solvents) which cannot be detected by chromatographic methods. For quantification purposes, only the qNMR value should be used since it is a direct/primary assay (i.e. an "absolute purity") with respect to the analyte.

Health & safety information:

Please refer to the Safety Data Sheet for detailed information about the nature of any hazard and appropriate precautions to be taken.

The purchaser must determine the suitability of this product for its particular use. Sigma-Aldrich Production GmbH makes no warranty of any kind, expressed or implied, other than its products meet all quality control standards set by Sigma-Aldrich Production GmbH. We do not guarantee that the product can be used for a special application. The expiry date assigns the time frame during which the unopened product is expected to remain within established specifications if stored under the conditions defined on the Certificate of Analysis.

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