Australian Government
Department of Industry, Science and Resources

National Measurement Institute

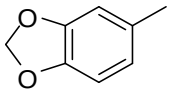
REFERENCE MATERIAL PRODUCT INFORMATION SHEET

NMIA D887b: 3,4-(Methylenedioxy)toluene

Report ID: D887b.2021.02

Chemical Formula: $C_8H_8O_2$

Molecular Weight: 136.1 g/mol



Property value

Batch No.	CAS No.	Purity by GC-FID
13-D-05	**62266-13-1**	**99.3 ± 0.02%**

IUPAC name: 5-methyl-1,3-benzodioxole.

Expiration of certification: The property values are valid till 12 August 2026, i.e. five years from the date of re-certification provided the **unopened** material is handled and stored in accordance with the recommendations below. The material as issued in the unopened container and stored as recommended below should be suitable for use beyond this date, subject to confirmation of batch stability from the issuing body. The expiry date/shelf life does not apply to sample bottles that have been opened. In such cases it is recommended that the end-user conduct their own in-house stability trials.

Description: Colourless liquid sourced from external supplier, and certified for identity and purity by NMIA. Packaged in amber glass bottles with a septum and crimped aluminium cap or screw top cap.

Intended use: This reference material is recommended for qualitative analysis only.

Instructions for use: Equilibrate the bottled material to room temperature before opening.

Recommended storage: When not in use this material should be stored at or below 25 ºC in a closed container in a dry, dark area.

Stability: This material has demonstrated stability over a minimum period of three years. The long-term stability of the compound in solution has not been examined.

Homogeneity assessment: The homogeneity of the material was assessed using purity assay by GC-FID on ten randomly selected 1-2 mg sub samples of the material. The material was judged to be sufficiently homogeneous at this level of sampling as the variation in analysis results between samples was not significantly different at a 95% confidence level from that observed on repeat analysis of the same sample.

Safety: Treat as a hazardous substance. Use appropriate work practices when handling to avoid skin or eye contact, ingestion or inhalation of dust. Refer to the provided safety data sheet.

S. R. Davies

Dr Stephen R. Davies,
Team Leader,
Chemical Reference Materials, NMI.
19 October 2022

This report supersedes any issued prior to 19 September 2022.

NATA Accreditation No. 198 / Corporate Site No. 14214.

Legal notice: Terms and Conditions associated with the provision of this reference material can be found on the NMIA website.

Characterisation Report:

The identity was confirmed by a range of spectroscopic techniques, NMR, IR and MS. Impurities of related structure were assessed by GC-FID.

Supporting evidence is provided by ^{1}H NMR spectroscopy and elemental microanalysis.

GC-FID:	Instrument:	Varian CP-3800
	Column:	TG-17MS/HP-5, 30 m × 0.32 mm I.D. × 0.25 μm
	Program:	60 °C (1 min), 5 °C/min to 150 °C, 30 °C/min to 280 °C (10 min)
	Injector:	250 °C
	Detector Temp:	320 °C
	Carrier:	Helium
	Split ratio:	20/1
	Relative peak area of main component:	
	Initial analysis:	Mean = 99.4%, s = 0.01% (10 sub samples in duplicate, February 2013)
	Re-analysis:	Mean = 99.4%, s = 0.01% (7 sub samples in duplicate, February 2014)
	Re-analysis:	Mean = 99.4%, s = 0.01% (5 sub samples in duplicate, December 2016)
	Re-analysis:	Mean = 99.3%, s = 0.02% (5 sub samples in duplicate, August 2021)

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ABN: 74 599 608 295
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Spectroscopic and other characterisation data

GC-MS:	Instrument:	Agilent 6890/5973
	Column:	TG-1MS, 30 m x 0.25 mm I.D. x 0.25 μm
	Program:	60 °C (1 min), 5 °C/min to 150 °C, 30 °C/min to 300 °C (3 min)
	Injector:	250 °C
	Split ratio:	20/1
	Transfer line temp:	280 °C
	Carrier:	Helium, 1.0 mL/min
	Scan range:	50-550 *m/z*
	The retention time of the parent compound is reported along with the major peaks in the mass spectrum. The latter are reported as mass/charge ratios and (in brackets) as a percentage relative to the base peak.	
	Parent (9.02 min):	135 (100), 78 (21), 77(20), 52 (10), 51 (14) *m/z*
IR:	Instrument:	Biorad FTS3000MX FT-IR
	Range:	4000-400 cm^{-1}, KBr powder
	Peaks:	2886, 1491, 1437, 1344, 1246, 1192, 1042, 936, 800, 755 cm^{-1}
^{1}H NMR:	Instrument:	Bruker Avance-400
	Field strength:	400 MHz
	Solvent:	$CDCl_3$ (7.26 ppm)
	Spectral data:	δ 2.28 (3H, s), 5.91 (2H, s), 6.62 (1H, m), 6.67 (1H, m), 6.71 (1H, d, *J* = 8.0 Hz) ppm
^{13}C NMR:	Instrument:	Bruker Gyro-300
	Field strength:	75 MHz
	Solvent:	$CDCl_3$ (77.2 ppm)
	Spectral data:	δ 21.1, 100.7, 108.0, 109.6, 121.5, 131.5, 145.3, 147.5 ppm
Microanalysis:	Found:	C = 70.8%; H = 6.0% (March, 2013)
	Calculated:	C = 70.6%; H = 5.9% (Calculated for $C_8H_8O_2$)