Australian Government
Department of Industry, Science and Resources

National Measurement Institute

NATA
WORLD RECOGNISED ACCREDITATION

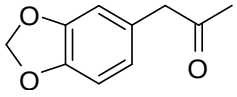
REFERENCE MATERIAL PRODUCT INFORMATION SHEET

NMIA D810b: 3,4-Methylenedioxyphenyl acetone

Report ID: D810b.2025.01

Chemical Formula: $C_{10}H_{10}O_3$

Molecular Weight: 178.2 g/mol



Property value

Batch No.	CAS No.	Purity estimate
08-D-08	**4676-39-5**	**92.7 ± 1.5%**

IUPAC name: 1-(1,3-Benzodioxol-5-yl)acetone

Expiration of certification: The property values are valid till 15 May 2028, three 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: Pale yellow oil prepared by synthesis, then certified for identity and purity by NMIA. Packaged in amber glass ampoule.

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 4 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 five 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.
27 May 2025

This report supersedes any issued prior to 27 May 2025.

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. The purity value was obtained by mass balance from a combination of traditional analytical techniques, including GC-FID and Karl Fisher analysis The purity value is calculated as per Equation 1.

Purity = (100 % - I_{ORG}) x (100 % - I_{VOL} – I_{NVR}) Equation 1

I_{ORG} = Organic impurities of related structure, I_{VOL} = volatile impurities, I_{NVR} = non-volatile residue.

Supporting evidence is provided by headspace GC-MS.

Warning: **This material is sensitive to the quality of the silanised glass liner when injected at elevated temperature (~ 250 ºC) into a GC instrument. Furthermore, this and previous batches of 3,4-methylenedioxyphenyl acetone have shown significant signs of degradation over time.**

GC-FID:	Instrument:	Varian CP-3800 or Agilent 8890
	Column:	VF-1 or HP-5, 30 m × 0.32 mm I.D. × 0.25 µm
	Program:	80 °C (1 min), 15°C/min to 100 °C, 20 °C/min to 300 °C (5 min)
	Injector:	150 - 180 °C
	Detector Temp:	320 °C
	Carrier:	Helium
	Split ratio:	20/1
	Relative peak area of the main component:	
	Initial analysis:	Mean = 98.2%, s = 0.3% (10 injections, February 2008)
	Re-analysis:	Mean = 95.4%, s = 0.05% (5 sub samples in duplicate, May 2011)
	Re-analysis:	Mean = 94.5%, s = 0.1% (5 sub samples in duplicate, April 2014)
	Re-analysis:	Mean = 92.8%, s = 0.1% (5 sub samples in duplicate, March 2017)
	Re-analysis:	Mean = 93.4%, s = 0.03% (5 sub samples in duplicate, May 2020)
	Re-analysis:	Mean = 93.5%, s = 0.07% (7 sub samples in duplicate, June 2023)
	Re-analysis:	Mean = 93.0%, s = 0.1% (5 sub samples in duplicate, May 2025)
Karl Fischer analysis:		Moisture content 0.2% mass fraction (June 2011) Moisture content 0.3% mass fraction (March 2014, 2017, 2020, 2023 and 2025)

Spectroscopic and other characterisation data

GC-MS:	Instrument:	Agilent 5890/5971
	Column:	ZB-5, 30 m x 0.25 mm I.D. x 0.25 μm
	Program:	60 °C (1 min), 10 °C/min to 250 °C (1 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 with the major peaks in the mass spectra. The latter are reported as mass/charge ratios and (in brackets) as a percentage relative to the base peak.	
	Parent (10.6 min):	178 (M^+, 30), 136 (11), 135 (100), 105 (5), 77 (17), 51 (8), 43 (6) *m/z*
IR:	Instrument:	Biorad WIN FTS3000 MX FTIR
	Range:	4000-400 cm^{-1}, NaCl plates
	Peaks:	2901, 1709, 1488, 1355, 1238, 1030, 924 cm^{-1}
^{1}H NMR:	Instrument:	Bruker DMX-600
	Field strength:	600 MHz
	Solvent:	$CDCl_3$ (7.26 ppm)
	Spectral data:	δ 2.14 (3H, s), 3.60 (2H, s), 5.94 (2H, s), 6.63 (1H, dd, *J* = 1.4, 7.9 Hz), 6.67 (1H, d, *J* = 1.4 Hz), 6.76 (1H, d, *J* = 7.9 Hz) ppm
^{13}C NMR:	Instrument:	Bruker DMX-600
	Field strength:	150 MHz
	Solvent:	$CDCl_3$ (77.2 ppm)
	Spectral data:	δ 29.0, 50.4, 101.0, 108.4, 109.7, 122.4, 127.7, 146.6, 147.8, 206.5 ppm