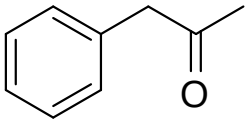
Australian Government
Department of Industry, Science and Resources

National Measurement Institute

NATA
WORLD RECOGNISED ACCREDITATION

REFERENCE MATERIAL PRODUCT INFORMATION SHEET

NMIA D868b: Benzyl methyl ketone



Report ID: D868b.2023.01

Chemical Formula: $C_{19}H_{10}O$

Molecular Weight: 134.2 g/mol

Property value

Batch No.	CAS No.	Organic Purity
09-D-12	**103-79-7**	**88.5 ± 0.1% by GC-FID**

The uncertainty has been calculated according to ISO Guide 35 and is stated at the 95% confidence limit (k = 2).

Synonyms: Phenylacetone, P2P

Expiration of certification: The property values are valid till 25 May 2028, 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: Light yellow liquid prepared by synthesis and certified for identity and purity by NMIA. Packaged in sealed amber ampoules.

Intended use: This reference material should be used for qualitative analysis only.

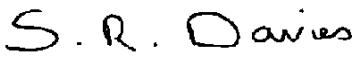
Instructions for use: Equilibrate the bottled material to room temperature before opening.

Recommended storage: When not in use this material should be stored at or below 4 °C in a closed container in a dry, dark area.

Stability: In the absence of long-term stability data the measurement uncertainty at the 95% coverage interval has been expanded to accommodate any potential change in the property value. The stability component has been estimated from stability trials conducted on similar materials by NMI Australia over the last 10 years. In the absence of long term stability data the measurement uncertainty at the 95% coverage interval has been expanded to accommodate any potential change in the property value. The stability component has been estimated from short term accelerated stability trials. 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.



Dr Stephen R. Davies,
Team Leader,
Chemical Reference Materials, NMI.
30 May 2023

This report supersedes any issued prior to 30 May 2023.

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

Characterisation Report:

The identity was confirmed by a range of spectroscopic techniques, NMR, IR and MS. The purity value was obtained by GC-FID. The purity value is calculated as per Equation 1.

Purity = (100 % - I_{ORG}) Equation 1

I_{ORG} = Organic impurities of related structure.

Supporting evidence is provided by elemental microanalysis.

Note: This material contains approximately 2.2% benzaldehyde, 0.2% benzyl alcohol, 1.8% benzyl acetate and 0.6% benzyl ethyl ketone.

<u>WARNING:</u> This material appears to be degrading over time. This should be taken into consideration when performing quantitative analysis.

GC-FID:	Instrument:	Varian CP-3800
	Column:	VF-1MS, 30 m × 0.32 mm I.D. × 0.25 ⌈m
	Program:	60 °C (1 min), 5 °C/min to 100 °C, 10 °C/min to 150 °C, 40 °C/min to 300 °C (1 min)
	Injector:	250 °C
	Detector Temp:	320 °C
	Carrier:	Helium
	Split ratio:	20/1
	Relative peak area of the main component:	
	Initial analysis:	Mean = 94.9%, s = 0.04% (10 sub samples in duplicate, April 2009)
	Re-analysis:	Mean = 94.0%, s = 0.06% (5 sub samples in duplicate, May 2010)
	Re-analysis:	Mean = 93.3%, s= 0.06% (5 sub samples in duplicate, May 2011)
GC-FID:	Instrument:	Agilent 6890
	Column:	HP-1, 30 m × 0.32 mm I.D. × 0.25 µm
	Program:	60 °C (1 min), 5 °C/min to 150 °C, 20°C/min to 300 °C (3 min)
	Injector:	250 °C
	Detector Temp:	320 °C
	Carrier:	Helium
	Split ratio:	20/1
	Relative peak area of the main component:	
	Initial analysis:	Mean = 92.2%, s = 0.007% (5 sub samples in duplicate, May 2012)
	Re-analysis:	Mean = 92.2%, s = 0.06% (5 sub samples in duplicate, March 2013)
	Re-analysis:	Mean = 92.1%, s = 0.06% (5 sub samples in duplicate, February 2014)
	Re-analysis:	Mean = 88.5%, s = 0.06% (5 sub samples in duplicate, January 2019)
	Re-analysis:	Mean = 88.4%, s = 0.1% (5 sub samples in duplicate, May 2023)
Thermogravimetric analysis:		Initial non volatile residue < 0.2 % mass fraction (April 2009) Volatile content not determined due to volatility of the material
Karl Fischer analysis:		Moisture content 1.1% mass fraction (April 2009, January 2019 and May 2023)

Spectroscopic and other characterisation data

GC-MS:	Instrument:	Agilent 6890/5973
	Column:	VF-1MS, 14.9 m × 0.25 mm I.D. × 0.25 µm
	Program:	60 °C (8 min), 5 °C/min to 150 °C (2 min), 40 °C/min to 250 °C (1 min)
	Injector:	250°C
	Transfer line temp:	280 °C
	Carrier:	Helium, 1.0 mL/min
	Split ratio:	20/1
	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.	
	9.2 min: 134 (M^+, 23), 91 (78), 65 (22), 43 (100) *m/z*	
IR:	Instrument:	Biorad FTS300MX FT-IR
	Range:	4000-700cm^{-1}, neat oil
	Peaks:	3031, 1710, 1357, 1228, 1158, 734 cm^{-1}
^{1}H NMR:	Instrument:	Bruker Gyro-300
	Field strength:	300 MHz
	Solvent:	$CDCl_3$ (7.26 ppm)
	Spectral data:	δ 2.16 (3H, s), 3.70 (2H, s), 7.19-7.23 (2H, m), 7.25-7.30 (1H, m), 7.31-7.37 (2H, m) ppm
^{13}C NMR:	Instrument:	Bruker Gyro-300
	Field strength:	75 MHz
	Solvent:	$CDCl_3$ (77.0 ppm)
	Spectral data:	δ 29.2, 51.0, 127.0, 128.7, 129.4, 134.2, 206.4 ppm
Microanalysis:	Found:	C = 78.7%; H = 7.1% (April 2009)
	Calc:	C = 80.6%; H = 7.5% (Calculated for $C_9H_{10}O$)