Australian Government
Department of Industry, Science and Resources

National Measurement Institute

NATA
WORLD RECOGNISED ACCREDITATION

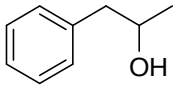
CERTIFIED REFERENCE MATERIAL CERTIFICATE OF ANALYSIS

NMIA D945: (±)-1-Phenyl-propan-2-ol

Report ID: D945.2020.03

Chemical Formula: $C_9H_{12}O$

Molecular Weight: 136.2 g/mol



Certified value

Batch No.	CAS No.	Purity (mass fraction)
09-D-24	**14898-87-4**	**88.1 ± 1.4%**

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

IUPAC name: 1-Phenyl-2-propanol.

Expiration of certification: The property values are valid till 9 April 2025, 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 prepared by synthesis, 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 certified reference material is suitable for use as a primary calibrator.

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.

Metrological traceability: The certified purity value is traceable to the SI unit for mass (kg) through Australian national standards via balance calibration. In the mass balance approach all impurities are quantified as a mass fraction and subtracted from 100%.

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 ten 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 seven 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.
20 September 2022

This report supersedes any issued prior to 20 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. The certified purity value was obtained by mass balance from a combination of traditional analytical techniques, including GC-FID, thermogravimetric analysis, Karl Fischer analysis and ^{1}H NMR spectroscopy. 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 qualitative elemental microanalysis.

Note: This material contains ca. 10.0% mass fraction benzyl alcohol.

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 100 °C (3 min), 10 °C/min to 150 °C (1 min), 30 °C/min to 300 °C (3 min)
	Injector:	250 °C
	Detector Temp:	320 °C
	Carrier:	Helium
	Split ratio:	20/1
	Relative mass fraction of the main component:	
	Initial analysis:	Mean = 90.0%, s = 0.09% (1 sub sample 7 injections, October 2009)
	Re-analysis:	Mean = 89.9%, s = 0.02% (7 sub samples in duplicate, January 2013)
	Re-analysis:	Mean = 89.5%, s = 0.04% (5 sub samples in duplicate, November 2015)
	Re-analysis:	Mean = 89.2%, s = 0.06% (5 sub samples in duplicate, April 2020)
Karl Fischer analysis:		Moisture content < 0.5% mass fraction (September 2009 and January 2013) Moisture content 1.1% mass fraction (November 2015) Moisture content 1.2% mass fraction (April 2020)
Thermogravimetric analysis:		Initial non-volatile residue < 0.1 % mass fraction (September 2009). Volatile content not determined due to volatility of the material

Spectroscopic and other characterisation data

GC-MS:	Instrument:	Agilent 6890N/5973
	Column:	DB35-MS, 30 m × 0.25 mm I.D. × 0.25 μm
	Program:	60 °C (1 min), 5 °C/min to 150 °C (1 min), 30 °C/min to 250 °C (1 min)
	Injector:	250 °C
	Split ratio:	Splitless
	Transfer line temp:	310 °C
	Carrier:	Helium, 1.2 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 (11.95 min):	136 (M^+, 2), 121 (3), 103 (3), 93 (8), 92 (100), 91 (64), 65 (9), 45 (15) *m/z*
TLC:	Conditions:	Kieselgel 60F_{254}. Hexane/ethyl acetate (8:2) Single spot observed, R_f =0.43. Visualisation with UV at 254 nm
IR:	Instrument:	Biorad FTS300MX FT-IR
	Range:	4000-400cm^{-1}, neat oil
	Peaks:	3333, 3028, 2970, 2928, 1497, 1454, 1373, 1207, 1119, 1080, 1038, 937, 837, 741, 702 cm^{-1}
^{1}H NMR:	Instrument:	Avance 400
	Field strength:	400 MHz
	Solvent:	$CDCl_3$
	Spectral data:	δ 1.26 (3H, d, *J* = 6.2 Hz), 1.93 (1H, d, *J* =3.6 Hz), 2.73 (1H, dd, *J* = 7.7, 13.4 Hz), 2.80 (1H, dd, *J* = 5.1, 13.4 Hz), 4.03 (1H, m), 7.20-7.40 (5H, m) ppm
		Benzyl alcohol was observed in the ^{1}H NMR at 10.0% mass fraction
^{13}C NMR:	Instrument:	Avance 400
	Field strength:	101 MHz
	Solvent:	$CDCl_3$ (77.0 ppm)
	Spectral data:	δ 22.6, 45.7, 68.7, 126.3, 128.4, 129.3, 138.5 ppm
Microanalysis:	Found:	C = 78.1%; H = 9.1 % (September 2009)
	Calculated:	C = 79.4 %; H = 8.9 % (Calculated for $C_9H_{12}O$)