Australian Government
Department of Industry, Science, Energy and Resources

National Measurement Institute

NATA
ACCREDITED FOR TECHNICAL COMPETENCE

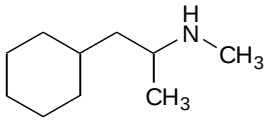
REFERENCE MATERIAL PRODUCT INFORMATION SHEET

NMIA M394: Propylhexedrine

Report ID: M394.2024.01

Chemical Formula: $C_{10}H_{21}N$

Molecular Weight: 155.3 g/mol



Property value

Batch No.	CAS No.	Purity by GC-FID
N/A	101-40-6	94.6 ± 0.2%

The uncertainty is based on the standard deviation of five analyses in duplicate and has been calculated according to ISO Guide 35 and is stated at the 95% confidence limit (k = 2).

IUPAC name: 1-Cyclohexyl-N-methyl-2-propanamine

Expiration of certification: The property values are valid till 20 September 2027, 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 flame sealed ampoule 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 ampoules 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 sourced from an external supplier, and certified for identity and purity by NMIA. Packaged in amber glass ampoules.

Intended use: This reference material is recommended for qualitative analysis only and is not intended for use as a calibrator. The material does not have certified reference material status as metrological traceability of the stated purity value to the SI unit for mass (kg) has not been established.

Instructions for use: Equilibrate the ampouled 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: 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 three 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.
23 September 2024

This report supersedes any issued prior to 23 September 2024

NATA logo notice: Accredited for compliance with ISO 17034. Accreditation No. 198 / Corporate Site No. 14214. The results of the tests, calibrations and/or measurements included in this document are traceable to Australian/national standards.

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 purity value was obtained by GC-FIDonly.

GC-FID:	Instrument:	Agilent 8890
	Column:	HP-1ms, 30 m × 0.32 mm I.D. × 0.25 μm
	Program:	70 °C (1 min), 8 °C/min to 200 °C, 20 °C/min to 300 °C (3 min)
	Injector:	180 °C
	Detector Temp:	320 °C
	Carrier:	Helium
	Split ratio:	20/1
	Relative peak area of the main component:	
	Initial analysis:	Mean = 94.8%, s = 0.1% (5 sub samples in duplicate, November 2021)
	Re- analysis:	Mean = 94.6%, s = 0.1% (3 sub samples in duplicate, November 2024)

Spectroscopic and other characterisation data

GC-MS:	Instrument:	HP6890/5973
	Column:	ZB-5 30 m x 0.25 mm I.D. x 0.3 μm
	Program:	60 °C (1 min), 8 °C/min to 100 °C, 12 °C/min to 250 °C (2 min)
	Injector:	180 °C
	Split ratio:	20/1
	Transfer line temp:	280 °C
	Carrier:	Helium, 1.0 mL/min
	Scan range:	50-500 *m/z*
	The retention time of the parent compound isreported 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 (8 min):	140 (5), 58 (100) *m/z*
IR:	Instrument:	Biorad FTS300MX FT-IR
	Range:	4000-400 cm^{-1}, KBr powder
	Peaks:	3678, 3294, 2922, 2849, 2790, 1666, 1631,1476,1342,1158,726 cm^{-1}
^{1}H NMR:	Instrument:	Bruker Avance III-500
	Field strength:	500 MHz
	Solvent:	$CDCl_3$ (7.3 ppm)
	Spectral data:	δ 0.80-0.91 (2H, m), 0.99 (3H, d, *J* = 6.3 Hz), 1.06-1.34 (6H, m), 1.58-1.70 (6H, m), 2.37(3H, s), 2.58 (1H, sextet) ppm
^{13}C NMR:	Instrument:	Bruker Avance III-300
	Field strength:	75 MHz
	Solvent:	$CDCl_3$ (77 ppm)
	Spectral data:	δ 20.2, 26.4, 26.5, 26.7, 33.6, 33.8, 34, 34.7, 45.2, 52.2 ppm