Australian Government
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National Measurement Institute

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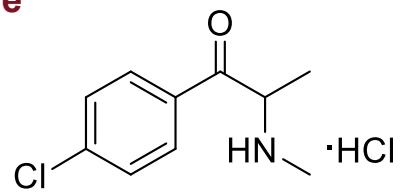
CERTIFIED REFERENCE MATERIAL CERTIFICATE OF ANALYSIS

NMIA D1093: 4-Chloromethcathinone Hydrochloride

Report ID: D1093.2026.01

Chemical Formula: $C_{10}H_{12}ClNO.HCl$

Molecular Weight: 234.1 g/mol (HCl), 197.7 g/mol (base)



Certified Value

Batch No.	CAS No.	Purity (mass fraction)
26-D-02	2319878-22-1 (HCl) 1225843-86-6 (base)	98.9 ± 2.0%

The uncertainty has been calculated according to ISO 33405 and is stated at the 95% confidence limit (k = 2.0).

IUPAC name: 1-(4-Chlorophenyl)-2-(methylamino)-1-propanone hydrochloride

Expiration of certification: The property values are valid till 27 July 2029, three years from the date of 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. The material will be re-tested periodically to ensure that the property values are still valid. In the event a product fails the stability trial, notification will be sent to all impacted customers.

Description: A white powder prepared by synthesis and certified for identity and purity by NMI Australia. Packaged in amber glass bottles with a septum and crimped aluminium 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 4 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 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 measurement uncertainty at the 95% confidence interval also includes a stability component determined from accelerated stability trials conducted at 40 ºC and 75% humidity for 14 days.

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.
25 August 2026

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.

$$\text{Purity} = (100\% - I_{ORG}) \times (100\% - I_{VOL} - I_{NVR}) \qquad \text{Equation 1}$$

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

Supporting evidence is provided by elemental microanalysis.

Warning: **This material is sensitive to the quality of the silanised glass liner when injected at elevated temperature (~ 100 ºC) into a GC instrument.**

GC-FID:	Instrument:	Varian CP-3800
	Column:	DB-17, 30 m × 0.32 mm I.D. × 0.25 μm
	Program:	60 °C (1 min), 10 °C/min to 100 °C, 15 °C/min to 280 °C (5 min)
	Injector:	100 °C
	Detector Temp:	320 °C
	Carrier:	Helium
	Split ratio:	20/1
	Relative mass fraction of the main componentas the derivatised (acetylated) compound:	
	Initial analysis:	Mean = 99.9%, s = 0.01% (10 sub samples in duplicate, July 2026)
Karl Fischer analysis:		Moisture content 0.9% mass fraction (July 2026)
Thermogravimetric analysis:		Non-volatile residue < 0.2% mass fraction (July 2026)

Spectroscopic and other characterisation data

GC-MS:	Parent compound:	
	Instrument:	Agilent 8890/5977B
	Column:	HP-5MS, 30 m × 0.25 mm I.D. × 0.25 μm
	Program:	90 °C (1 min), 15 °C/min to 240 °C, 25 °C/min to 300 °C (4 min)
	Injector:	250 °C
	Split ratio:	20/1
	Transfer line temp:	280 °C
	Carrier:	Helium, 1.0 mL/min
	Scan range:	40–350 *m/z*
	The retention time of 4-chloromethcathinone free base 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 (8.2 min):	141 (7), 139 (22), 111 (18), 75 (15), 58 (100), 56 (14), 44 (69), 43 (16), 42 (9) *m/z*
ESI-MS:	Instrument:	Shimadzu LC-TQ-MS 8045
	Operation:	Direct infusion at 10 μL/min
	Mobile Phase:	Isocratic Acetonitrile (65%) / Milli-Q water (0.2% formic acid)
	Flow Rate :	1.0 mL/min
	Ionisation mode:	Electrospray positive ion
	Interface voltage:	4.0 kV
	Peak:	200 $[M(^{37}Cl) + H]^+$, 198 $[M(^{35}Cl) + H]^+$ *m/z*
TLC:	Conditions:	Kieselgel 60 F_{254}. $CHCl_3/CH_3OH$ (1:1, *v/v*) Single spot observed, R_f = 0.57. Visualisation with UV at 254 nm.
FTIR:	Instrument:	Bruker ALPHA II PLATINUM-ATR
	Range:	4000−350 cm^{-1}, neat
	Peaks:	2913, 2696, 2462, 1689, 1588, 1470, 1401, 1297, 1092, 976, 911, 844, 745, 531 cm^{-1}
^{1}H-NMR:	Instrument:	Bruker Avance III-500
	Field strength:	500 MHz
	Solvent:	Acetic Acid-d_4 (2.04 ppm)
	Spectral data:	δ 1.67 (3H, d, *J* = 7.3 Hz), 2.87 (3H, s), 5.23 (1H, q, *J* = 7.2, 7.3 Hz), 7.59 (2H, app. d, *J* = 8.7 Hz), 8.03 (2H, app. d, *J* = 8.7 Hz) ppm
^{13}C-NMR:	Instrument:	Bruker Avance III-500
	Field strength:	126 MHz
	Solvent:	Acetic Acid-d_4 (20 ppm)
	Spectral data:	δ 16.3, 32.4, 60.7, 130.5, 131.6, 132.4, 142.2, 195.9 ppm
Melting point (Hot Stage):		202–207 °C
Microanalysis:	Found:	C = 51.3%; H = 5.7%; N = 6.0% (July 2026)
	Calculated:	C = 51.0%; H = 5.7%; N = 5.8% (Calculated for $C_{10}H_{12}ClNO{\cdot}HCl$)