

Certificate of Analysis

Reference Substance

Methylpentynol

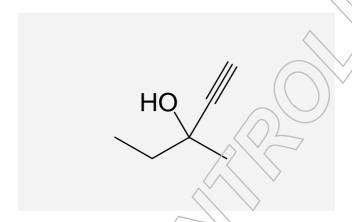
CAS Number:

Catalogue Number: LGCFOR1275.53

Long-term Storage: 2 to 8 °C, dark

Appearance: colourless liquid

Assay 'as is': 99.6 %



[77-75-8]

Date of shipment: 2016-May-20

This certificate is valid for one year from the date of shipment provided the substance is stored under the recommended conditions.

Release Date: 2011-07-15

LGC GmbH

Dr. Sabine Schröder Product Release







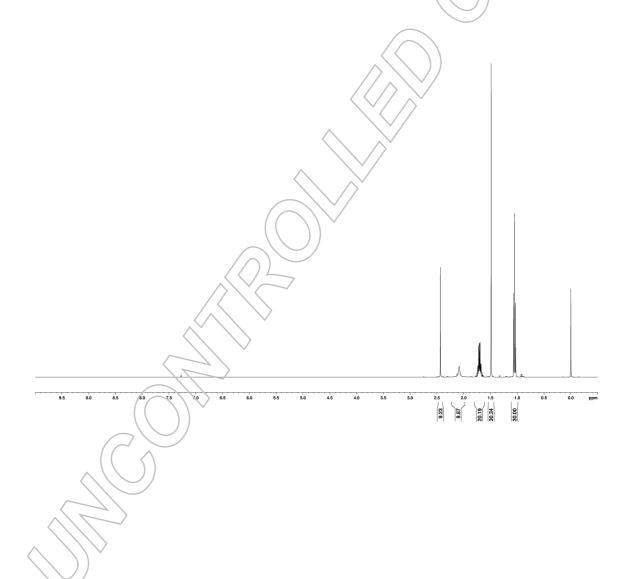
I. Identity

The identity of the reference substance was established by following analyses.

la. ¹H-NMR Spectrum

Conditions: 400 MHz, CDCl₃

The structure is confirmed with the signals of the spectrum and their interpretation.

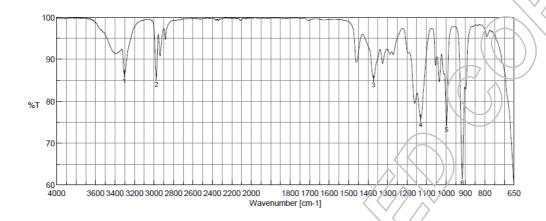






lb. IR Spectrum

Method: Attenuated Total Reflection Fourier Transform Infrared (ATR-FTIR) Spectroscopy



Result of Peak Picking
No. Position Intensity
1 3304.43 86.4841
2 2974.66 85.6468
3 1372.1 85.4373
4 1129.12 75.9529
5 996.053 74.891
6 916.022 62.173

The signals of the IR spectrum and their interpretation are consistent with the structural formula.

II. Purity

The purity of the reference substance was analysed by headspace gas chromatography (GC-FID).

GC Conditions:

Column: Oven Program: Detector:

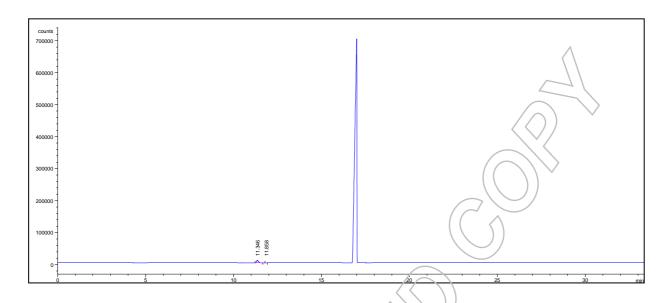
DB 624 splitless Injection, 150 °C Initial Temp.: 38 °C for 6 min FID

30 m x 0.32 mm x 1.8 µm Nitrogen 54 ml/min Heating Rate: 15 °C/min Hydrogen 35 ml/min

Compressed air 350 ml/min Final Temp.: 200 °C 250 °C







Area Percent Report - Sorted by Signal

Pk#	Retention Time	Area.	Area %	
1	11.35	54106.59	99.65	
2	11.86	190.52	0.35	
Totals		54297.11	100.00	

For the calculation the air peaks were ignored. The content of the analyte was determined as ratio of the peak area of the analyte and the cumulative areas of the purities, added up to 100 %.

Results:

Average

99.67 %

Number of results

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Standard deviation

0.05 %





III. Water Content

Method: Karl Fischer titration

Results:

IV. Residual Solvents

Method: 1H-NMR

No significant amounts of residual solvents were detected (< 0.05 %)

V. Final Result

Residual solvents n. d. (not detected)

Assay (100 % method) 99.58 %

The assay is assessed to be 99.6 % 'as is'

The assay 'as is' is equivalent to the assay based on the not anhydrous and not dried substance respectively.

¹ The calculation of the 100 % method follows the formula:

Assay (%) = (100 % - KF - RES) * $\frac{Purity GC (\%)}{100 \%}$

Water (KF) and Residual solvents (RES) are considered as absolute contributions, GC purity is considered as relative contribution.

LGCFOR1275.53 Lot Number 6543

Excellence through measurement