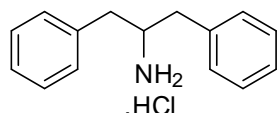




REFERENCE MATERIAL ANALYSIS REPORT

Report ID: D971.2016.01

Compound Name:  $\alpha$ -Benzylphenethylamine hydrochloride Description: White powder  
Collection number: D971 Batch number: 11-D-12  
Chemical Formula:  $C_{15}H_{17}N.HCl$  Molecular Weight: 247.8 (HCl), 211.3 (base)  
CAS Registry Number: 7763-96-4 (HCl), 4275-43-8 (base) Release date: July 2011  
Structure:



Synonyms: 1,3-Diphenyl-2-propylamine hydrochloride  
2-Amino-1,3-diphenylpropane hydrochloride  
 $\beta,\beta'$ -Diphenylisopropylamine hydrochloride  
 $\alpha$ -(Phenylmethyl)-benzeneethanamine hydrochloride

Purity (mass fraction):  $99.8 \pm 1.3\%$  (95% coverage interval)

**This reference material has NOT been extensively quantified by the Chemical Reference Materials team at NMI and should be considered for use in qualitative analysis only.**

The purity value was obtained from a combination of traditional analytical techniques, by subtraction from 100% of total impurities by GC-FID, thermogravimetric analysis, Karl Fischer analysis, and <sup>1</sup>H NMR spectroscopy. Supporting evidence is provided by headspace GC-MS analysis of occluded solvents and elemental microanalysis.

GC-FID: Instrument: Varian CP-3800  
Column: VF-1MS, 30 m  $\times$  0.32 mm I.D.  $\times$  0.25  $\mu$ m  
Program: 120  $^{\circ}$ C (1 min), 20  $^{\circ}$ C/min to 250  $^{\circ}$ C (2 min), 30  $^{\circ}$ C/min to 300  $^{\circ}$ C (3 min)  
Injector: 250  $^{\circ}$ C Detector Temp: 320  $^{\circ}$ C  
Carrier: Helium Split ratio: 20/1  
Relative peak area of main component as the free base:  
Initial analysis: Mean = 99.97%, s = 0.03% (10 sub samples in duplicate, July 2011)  
Re-analysis: Mean = 99.96%, s = 0.02% (5 sub samples in duplicate, July 2012)

GC-FID: Instrument: Varian CP-3800  
Column: HP-5, 30.0 m  $\times$  0.32 mm I.D.  $\times$  0.25  $\mu$ m  
Program: 120  $^{\circ}$ C (1 min), 20  $^{\circ}$ C/min to 250  $^{\circ}$ C (2 min), 30  $^{\circ}$ C/min to 300  $^{\circ}$ C (3 min)  
Injector: 250  $^{\circ}$ C Detector Temp: 320  $^{\circ}$ C  
Carrier: Helium Split ratio: 20/1  
Relative peak area of main component as the free base:  
Initial analysis: Mean = 99.98%, s = 0.02% (10 sub samples in duplicate, July 2011)  
Re-analysis: Mean = 99.97%, s = 0.007% (5 sub samples in duplicate, May 2016)

Thermogravimetric analysis: The volatile content could not be determined using thermogravimetric analysis. Non volatile residue < 0.1% mass fraction (August 2011).

Karl Fischer analysis: Moisture content 0.1% mass fraction (August 2011 and July 2012)  
Moisture content < 0.1% mass fraction (May 2016)





### Expiration of certification

The property values are valid till 26<sup>th</sup> May 2021, 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.

The long-term stability of the compound in solution has not been examined.

This material has been given a shelf life of five years from the date of re-certification.

This material has demonstrated stability over a minimum period of five years. The measurement uncertainty at the 95% coverage interval includes a stability component which has been estimated from annual stability trials.

### 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.

### Recommended storage

When not in use this material should be stored at or below 25 °C in a closed container in a dry, dark area.

### Intended Use

For *in vitro* laboratory analysis only.

### Caution

Treat as hazardous substance. Use appropriate work practices when handling to avoid skin or eye contact, ingestion or inhalation of dust.

### Legal notice

Neither NMI nor any person acting on NMI's behalf assumes any liability with respect to the use of, or for damages resulting from the use of, this reference material or the information contained in this certificate.

Authorised by:

S. R. Davies

Dr Stephen R Davies  
Team Leader,  
Chemical Reference Materials, NMI  
Dated: 1<sup>st</sup> June 2016

Characterisation data and property values specified in this report supersede all reports issued prior to 1<sup>st</sup> June 2016.



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