National Measurement Institute



REFERENCE MATERIAL PRODUCT INFORMATION SHEET

NMIA P1642: Dimethoate

Report ID: P1642.2021.02

Chemical Formula: $C_5H_{12}NO_3PS_2$

Molecular Weight: 229.3 g/mol

Property value

Batch No.	CAS No.	Purity estimate
00-AV-01	60-51-5	99.4%

IUPAC name: (1Z)-2-[(Dimethoxyphosphorothioyl)sulfanyl]-N-methylethanimidic acid

Expiration of certification: The property values are valid till 16 September 2031, i.e. ten 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: White crystals sourced from an external supplier, 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 reference material is recommended for qualitative analysis only.

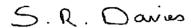
Instructions for use: Equilibrate the bottled material to room temperature before opening.

Recommended storage: When not in use this material should be stored at or below 4 °C in a closed container in a dry, dark area.

Stability: This material has demonstrated stability over a minimum period of 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.



Dr Stephen R. Davies, Team Leader, Chemical Reference Materials, NMI. 6 September 2022

This report supersedes any issued prior to 6 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 purity value was obtained by mass balance from a combination of traditional analytical techniques, including GC-FID, thermogravimetric analysis, Karl Fischer analysis and ¹H NMR spectroscopy. The purity value is calculated as per Equation 1.

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

Equation 1

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

Supporting evidence is provided by elemental microanalysis.

GC-FID: Instrument: Agilent 6890 or 8890

Column: HP-1 Capillary, 30 m \times 0.32 mm I.D. \times 0.25 μ m

Program: 120 °C (1 min), 10 °C/min to 220 °C

Injector: 250 °C

Detector Temp: 320 °C

Carrier: Helium

Split ratio: 20/1

Relative peak area of the main component:

Initial analysis: Mean = 99.9%, s = 0.07% (8 sub samples in duplicate, June 1999) Re-analysis: Mean = 99.7%, s = 0.03% (5 sub samples in duplicate, November 2011) Re-analysis: Mean = 99.6%, s = 0.03% (5 sub samples in duplicate, September 2021)

HPLC: No impurity peaks were detected in any of the samples using a 20 μ l injection volume of a 4000 μ g/ml solution.

Peak area percentage of total > 99.9% (7 replicates)

Column: Waters Nova-Pak C18, 5 μ m (150 mm \times 3.9 mm)

Mobile Phase: Acetonitrile/ Water (20:80)

Flow Rate: 0.8 mL/min
Detector: Refractive index

DSC: Quantitative purity assay was carried out on 2-3 mg quantities of P1642:

Instrument: Perkin-Elmer Pyris 1.

Temperature program: 19 °C, hold 1min, 0.7 °C/min to 58 °C.

Results: Purity = 98.4% mol/mol, s = 0.35% (8 samples)

Karl Fischer analysis: Moisture content 0.2% mass fraction (November 2011 & September 2021)

Thermogravimetric analysis: Non-volatile residue < 0.2% mass fraction (October 2005)