



National Institute of Standards & Technology

Report of Investigation

Reference Material 8182

Fatty Acid Methyl Esters in 2,2,4-Trimethylpentane

This Reference Material (RM) is a solution of 26 fatty acid methyl esters (FAMES) in 2,2,4-trimethylpentane. This RM is intended for use in evaluating analytical methods and chromatographic instrumentation used for the determination of FAMES. A unit of RM 8182 consists of five 2 mL ampoules, each containing approximately 1.2 mL of solution.

Due to the original NIST fatty acid determinations in SRM 2377 not being sufficiently traceable to the International System of Units (SI), SRM 2377 no longer meets international quality standards (ISO 17034) for serving as a certified reference material. However, the material continues to meet ISO 17034 standards as a reference material and is thus being offered as RM 8182.

Non-Certified Mass Fractions of Constituents: The non-certified mass fraction values and estimated uncertainties for the 26 FAMES are given in Table 1 along with the Chemical Abstract Service (CAS) Registry Numbers. The non-certified mass fraction values are based on masses used in the gravimetric preparation of this solution and from the analytical results determined by using gas chromatography. Non-certified values represent best estimates of the true value; however, the values do not meet the NIST criteria for certification and are provided with associated uncertainties that may reflect only measurement precision, may not include all sources of uncertainty, or may reflect a lack of sufficient statistical agreement among multiple analytical methods [1]. Non-certified values are traceable to the measurement processes and standards used by NIST.

Period of Validity: RM 8182 is valid, within the measurement uncertainty specified, until **30 June 2026**, provided the RM is handled and stored in accordance with instructions given in this Report of Investigation (see "Instructions for Handling, Storage, and Use"). This report is nullified if the RM is damaged, contaminated, or otherwise modified.

Maintenance of Non-Certified Value: NIST will monitor this material to the end of its period of validity. If substantive technical changes occur that affect the non-certified values during this period, NIST will update this Report of Investigation and notify the purchaser. Registration (see attached sheet or register online) will facilitate notification. However, before making use of any of the values delivered by this material, please check for the most recent documentation on the NIST SRM website at <https://www.nist.gov/srm>.

Overall direction and coordination of technical measurements leading to value assignment were performed by L.C. Sander of the NIST Chemical Sciences Division, and M.M. Schantz, formerly of NIST.

Preparation and analytical measurements of the RM were performed by M.M. Schantz, formerly of NIST. Statistical consultation was provided by S.D. Leigh, formerly of NIST.

Support aspects involved in the issuance of this RM were coordinated through the NIST Office of Reference Materials.

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INSTRUCTIONS FOR HANDLING, STORAGE, AND USE

Handling: This material should be handled with care. Use proper disposal methods.

Storage: The material should be stored under refrigeration (0 °C to 4 °C), in an unopened ampoule, until required for use.

Use: Prior to removal of a test portion for analysis, the contents of an ampoule should be allowed to warm to room temperature and mixed thoroughly. Sample aliquots for analysis should be withdrawn at 20 °C to 25 °C **immediately** after opening the ampoules and should be processed without delay for the non-certified values in Table 1 to be valid within the stated uncertainties. Because of the volatility of 2,2,4-trimethylpentane, non-certified values are not applicable to material stored in ampoules that have been opened for more than 5 minutes, even if they are resealed.

PREPARATION AND ANALYSIS⁽¹⁾

The compounds used in the preparation of this RM were obtained from commercial sources. The solution was prepared at NIST by weighing and combining the individual compounds and 2,2,4-trimethylpentane. The weighed components were added to the 2,2,4-trimethylpentane and mixed overnight. The total mass of this solution was measured, and the mass fractions were calculated. These gravimetric concentrations were adjusted for the purity estimation of each component, which was determined by using capillary gas chromatography with two stationary phases of different polarities. The bulk solution was chilled slightly, and 1.2 mL aliquots were dispensed into 2-milliliter glass ampoules, which were flushed with argon then flame-sealed.

Aliquots from nine ampoules, selected using a random stratified sampling scheme, were analyzed in duplicate by using capillary gas chromatography with flame ionization detection (GC-FID) on a relatively polar nonbonded, biscyanopropyl polysiloxane phase (SP 2560, 100 m × 0.25 mm id, 0.25 µm film thickness, Supelco, Bellefonte, PA). The internal standard solution added to each sample for quantification purposes contained methyl tridecanoate, methyl heneicosanoate, and methyl octacosanoate. Calibration solutions consisting of weighed amounts of the 26 FAMES and the internal standard compounds in 2,2,4-trimethylpentane were chromatographically analyzed to determine analyte response factors.

⁽¹⁾Certain commercial equipment, instruments or materials are identified in this report to adequately specify the experimental procedure. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

Table 1. Non-Certified Mass Fraction Values of FAMES

FAME	CAS Registry No. ^(a)	Mass Fraction (mg/g) ^(b)
Octanoic Acid Methyl Ester (Caprylic Acid Methyl Ester)	111-11-5	7.286 ± 0.054
Decanoic Acid Methyl Ester (Capric Acid Methyl Ester)	110-42-9	7.499 ± 0.058
Dodecanoic Acid Methyl Ester (Lauric Acid Methyl Ester)	111-82-0	7.93 ± 0.11
Tetradecanoic Acid Methyl Ester (Myristic Acid Methyl Ester)	124-10-7	7.11 ± 0.13
Hexadecanoic Acid Methyl Ester (Palmitic Acid Methyl Ester)	112-39-0	7.38 ± 0.32
Octadecanoic Acid Methyl Ester (Stearic Acid Methyl Ester)	112-61-8	7.68 ± 0.12
Eicosanoic Acid Methyl Ester (Arachidic Methyl Ester)	1120-28-1	3.66 ± 0.21
Docosanoic Acid Methyl Ester (Behenic Acid Methyl Ester)	929-77-1	4.28 ± 0.10
Tetracosanoic Acid Methyl Ester (Lignoceric acid methyl ester)	2442-49-1	1.807 ± 0.081
9-Tetradecenoic Acid Methyl Ester (Myristoleic Acid Methyl Ester)	56219-06-8	1.894 ± 0.033
9-Hexadecenoic Acid Methyl Ester (Palmitoleic Acid Methyl Ester)	1120-25-8	5.031 ± 0.039
9-Octadecenoic Acid Methyl Ester (Oleic Acid Methyl Ester)	112-62-9	7.01 ± 0.31
9- <i>trans</i> -Octadecenoic Acid Methyl Ester (Elaidic Acid Methyl Ester)	1937-62-8	2.02 ± 0.18
11-Octadecenoic Acid Methyl Ester (Vaccenic Acid Methyl Ester)	1937-63-9	2.31 ± 0.14
11- <i>trans</i> -Octadecenoic Acid Methyl Ester (<i>trans</i> -Vaccenic Acid Methyl Ester)	6198-58-9	2.368 ± 0.047
9,12-Octadecadienoic Acid Methyl Ester (Linoleic Acid Methyl Ester)	112-63-0	7.33 ± 0.14
9- <i>trans</i> ,12- <i>trans</i> -Octadecadienoic Acid Methyl Ester (Linoelaidic Acid Methyl Ester)	2566-97-4	2.046 ± 0.015
9,12,15-Octadecatrienoic Acid Methyl Ester (<i>alpha</i> -Linolenic Acid Methyl Ester)	301-00-8	4.26 ± 0.26
6,9,12-Octadecatrienoic Acid Methyl Ester (<i>gamma</i> -Linolenic Acid Methyl Ester)	16326-32-2	1.796 ± 0.052
11-Eicosenoic Acid Methyl Ester (Gondoic Acid Methyl Ester)	2390-09-2	1.919 ± 0.081
5,8,11,14-Eicosatetraenoic Acid Methyl Ester (Arachidonic Acid Methyl Ester)	2566-89-4	1.511 ± 0.063
5,8,11,14,17-Eicosapentaenoic Acid Methyl Ester (EPA Methyl Ester)	2734-47-6	1.526 ± 0.068
7,10,13,16,19-Docosapentaenoic Acid Methyl Ester (DPA Methyl Ester)	108698-02-8	1.426 ± 0.030
4,7,10,13,16,19-Docosahexaenoic Acid Methyl Ester (DHA Methyl Ester)	2566-90-7	1.621 ± 0.082
13-Docosenoic Acid Methyl Ester (Erucic Acid Methyl Ester)	1120-34-9	2.204 ± 0.083
15-Tetracosenoic Acid Methyl Ester (Nervonic Acid Methyl Ester)	2733-88-2	1.74 ± 0.011

^(a) Chemical Abstracts, Fourteenth Collective Index. Index Guide, American Chemical Society, Columbus, Ohio 2001.

^(b) The non-certified value is a weighted mean of the mass fractions determined by gravimetric and chromatographic measurements [2], corrected for purity. The uncertainty listed with each value is an expanded uncertainty about the mean [3,4], with coverage factor 2 (approximately 95 % confidence), calculated by combining a between-method variance incorporating inter-method variance following the ISO/JCGM Guide [5].

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