National Institute of Standards & Technology

Certificate of Analysis

Standard Reference Material® 2214

Isooctane
(2, 2, 4-Trimethylpentane)
Liquid Density

This Standard Reference Material (SRM) is intended for use as a calibration material for densimeters. SRM 2214 is a high purity liquid isooctane characterized for density, ρ(T), in the temperature range of 15.000 °C to 25.000 °C. A unit consists of four flame-sealed glass ampoules each, containing approximately 5 mL of isooctane. Certified values and uncertainties are given in Table 1 for the liquid density at three sample temperatures.

Table 1. Certified Values and Uncertainties of SRM 2214 at Three Sample Temperatures

Temperature, °C	Density, kg/m^3
15.000	695.969 ± 0.035
20.000	691.872 ± 0.035
25.000	687.753 ± 0.035

The interpolation equation, valid between 15.000 °C and 25.000 °C, is

$$?(T) = 691.872\ \left[1 - 1.18752\ \times 10^{-3}(T-20) - 6.2516\ \times 10^{-7}(T-20)^2\right] \qquad (1)$$

where T is in the sample temperature in °C.

Certified Values and Uncertainties: The certified values are based on instrumental measurements directly traceable to a definitive method for density determination. The uncertainties are approximate 95 % prediction intervals for isooctane density that incorporate standard uncertainties for random measurement variability, day-to-day measurement variability, variability in isooctane density from ampoule-to-ampoule, and uncertainties in instrument calibration. The true density of each ampoule of this material will lie within the associated prediction interval with high probability at the certified temperatures. The end points of the prediction interval are based on an expanded uncertainty for isooctane density with a coverage factor of k = 2.13. The coverage factor was obtained from the Student's t-distribution with 15.2 effective degrees of freedom [1].

Expiration of Certification: The certification of this SRM is valid indefinitely within the measurement uncertainties specified, provided that the SRM is used in accordance with the instructions given in this certificate. However, the certification will be nullified if the SRM is modified or contaminated.

Characterization of this SRM was performed by J.F. Houser and V.E. Bean of the NIST Process Measurements Division.

Statistical analysis was provided by W.F. Guthrie of the NIST Statistical Engineering Division.

The support aspects involved in the preparation, certification, and issuance of this SRM were coordinated through the NIST Standard Reference Materials Program by J.C. Colbert.

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Certificate Issue Date: 20 February 2001

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The overall direction and coordination of the technical measurements leading to certification were provided by V.E. Bean of the NIST Process Measurements Division.

Source and Preparation of Material: The isooctane used to produce this SRM was obtained from a commercial source. It was flame-sealed in glass ampoules, each containing approximately 5 mL of the liquid.

Storage and Handling: The unopened ampoules comprising the SRM must be stored at normal ambient temperature.

Instructions for Use: The sample tube of the densimeter should be cleaned according to the manufacturer's instructions. When an ampoule is to be opened, that area of the stem where the prescored band is located (~5 mm below the encircling metallic band) should be carefully wiped with a clean, damp cloth and the body of the ampoule wrapped in absorbent material. Then, holding the ampoule steady and with thumb and forefinger grasping the stem at the metallic band, **minimal** thumb pressure should be applied to the stem to snap it. (Correctly done, the stem should break easily where prescored. Use of a metal file to break the stem is **NOT** recommended.) After opening the ampoule, the entire contents should be transferred immediately to another container and dilutions made in accordance with the following subsections. The isooctane should be injected into the sample tube according to the densimeter manufacturer's instructions. A plastic syringe should **NOT** be used as the plastic may be soluble in isooctane.

The uncertainty in results from the interpolation equation will depend upon the uncertainty in the user's temperature measurements. The standard uncertainty, u_c, for the interpolation equation can be approximately expressed as

$$u_c = \left\{ (s_{\rho 20})^2 + \left[\rho_{20}(T-20)s_\beta\right]^2 + \left[\rho_{20}(T-20)^2 s_\gamma\right]^2 + (\rho_{20}\beta s_T)^2 \right\}^{\frac{1}{2}} \qquad (2)$$

where:

$s_{\rho 20}$ is the expanded uncertainty for the density at 20 °C from Table 1, divided by its coverage factor of k = 2.13.

ρ_{20} is the density at 20 °C from Table 1.

T is the sample temperature measured by the user, in °C.

s_β is the standard uncertainty for the first order coefficient in the interpolation equation obtained from the regression calculation and is equal to 1.06×10^{-7} with 6 degrees of freedom.

s_γ is the standard uncertainty for the second order coefficient in the interpolation equation obtained from the regression calculation and is equal to 3.66×10^{-8} with 6 degrees of freedom.

β is the first order coefficient in the interpolation equation.

s_T is the uncertainty for the user's sample temperature measurements, in °C.

The expanded uncertainty U, for the interpolation equation can be approximately expressed as $U = 2u_c$, using a coverage factor of k = 2 (see note after equation 3).

Using the fact that the uncertainty from the linear regression will be greatest for T = 15 °C and T = 25 °C, with the substitution of values, the expanded uncertainty, U, becomes

$$U = 2\left[3.04 \times 10^{-4} + 0.8(s_T)^2\right]^{\frac{1}{2}} \qquad (3)$$

NOTE: If the uncertainty of the user's sample temperature measurement is not based on a large number of effective degrees of freedom (>30), then the user should replace the coverage factor, k = 2, in equations 2 and 3 with a coverage factor obtained from the Student's *t*-distribution using the methods in the ISO Guide [1].

Table 2. Expanded Uncertainties from the Interpolation Equation for Some Examples of Uncertainties in Sample Temperature Measurement

s_T, °C	U, kg/m^3
0.001	0.035
0.01	0.039
0.1	0.203

REFERENCE

[1] *Guide to the Expression of Uncertainty in Measurement*, ISBN 92-67-10188-9 1st Ed., ISO, Geneva, Switzerland, (1993); see also Taylor, B.N. and Kuyatt, C.E., "Guidelines for Evaluating and Expressing Uncertainty of NIST Measurement Results," NIST Technical Note 1297, U.S. Government Printing Office, Washington DC, (1994); available at http://physics.nist.gov/Pubs/.

Users of this SRM should ensure that the certificate in their possession is current. This can be accomplished by contacting the SRM Program at: telephone (301) 975-6776; fax (301) 926-4751; e-mail srminfo@nist.gov; or via the Internet http://www.nist.gov/srm.