
**Water quality — Determination of
volatile organic compounds in water
— Method using headspace solid-
phase micro-extraction (HS-SPME)
followed by gas chromatography-mass
spectrometry (GC-MS)**

*Qualité de l'eau — Détermination de composés organiques volatils
dans l'eau — Méthode utilisant une micro-extraction en phase solide
(MEPS) de l'espace de tête suivie d'une chromatographie en phase
gazeuse-spectrométrie de masse (CG-SM)*



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Foreword

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For an explanation on the meaning of ISO specific terms and expressions related to conformity assessment, as well as information about ISO's adherence to the WTO principles in the Technical Barriers to Trade (TBT) see the following URL: [Foreword - Supplementary information](#)

The committee responsible for this document is ISO/TC 147, *Water quality*, Subcommittee SC 2, *Physical, chemical and biochemical methods*.

Introduction

Volatile organic compounds (VOCs) are often found in the manufacturing processes of paints, adhesives, petroleum products, pharmaceuticals, and refrigerants. Some are used as gasoline additives, solvents, hydraulic fluids, and dry-cleaning agents. This group of compounds belongs to the group of anthropogenic chemicals. VOC contamination of water resources is a human-health concern because many are toxic and are known or suspected human carcinogens.

For the determination of VOCs, several published procedures are available (see References [4],[5],[6],[7],[9],[12],[13], and [14]).

Water quality — Determination of volatile organic compounds in water — Method using headspace solid-phase micro-extraction (HS-SPME) followed by gas chromatography-mass spectrometry (GC-MS)

WARNING — Persons using this International Standard should be familiar with normal laboratory practice. This International Standard does not purport to address all of the safety problems, if any, associated with its use. It is the responsibility of the user to establish appropriate safety and health practices and to ensure compliance with any national regulatory conditions.

IMPORTANT — It is absolutely essential that tests conducted in accordance with this International Standard be carried out by suitably qualified staff.

1 Scope

This International Standard specifies a method for the determination of volatile organic compounds (see [Table 1](#)). This comprises, for example, halogenated hydrocarbons, trihalogenated methanes, gasoline components (such as BTEX, MTBE, and ETBE), naphthalene, 2-ethyl-4-methyl-1,3-dioxolane, and highly odorous substances like geosmin and 2-methylisoborneol in drinking water, ground water, surface water, and treated waste water, by means of headspace solid-phase micro-extraction (HS-SPME) followed by gas chromatography-mass spectrometry (GC-MS). The limit of determination depends on the matrix, on the specific compound to be analysed, and on the sensitivity of the mass spectrometer. For most compounds to which this International Standard applies, it is at least 0,01 µg/l. Validation data related to a concentration range between 0,02 µg/l and 2,6 µg/l have been demonstrated in an interlaboratory trial. Additional validation data derived from standardization work show applicability of the method within a concentration range from 0,01 µg/l to 100 µg/l of individual substances. All determinations are performed on small sample amounts (e.g. sample volumes of 10 ml).

This method may be applicable to other compounds not explicitly covered by this International Standard or to other types of water. However, it is necessary to demonstrate the applicability for each case.

Table 1 — Volatile organic compounds determinable by this method

Name	Molecular formula	CAS registry no. ^d	Molar mass g/mol	Density kg/l
<i>tert</i> -amyl methyl ether (TAME)	C ₆ H ₁₄ O	994-05-8	102,17	0,76
benzene	C ₆ H ₆	71-43-2	78,12	0,88
bromobenzene	C ₆ H ₅ Br	108-86-1	157,01	1,50
bromochloromethane	CH ₂ BrCl	74-97-5	129,38	1,99
bromodichloromethane	CHBrCl ₂	75-27-4	163,83	1,98
<i>n</i> -butylbenzene	C ₁₀ H ₁₄	104-51-8	134,22	0,86
<i>sec</i> -butylbenzene	C ₁₀ H ₁₄	135-98-8	134,22	0,86
<i>tert</i> -butylbenzene	C ₁₀ H ₁₄	98-06-6	134,22	0,87
chlorobenzene	C ₆ H ₅ Cl	108-90-7	112,56	1,11

^a Signals of substances may overlap in chromatograms as they might co-elute.

^b Density of liquid at boiling point (-13,4 °C)

^c Refer to [Tables F.1](#) and [F.2](#) for validation data and additional information.

^d CAS: Chemical Abstracts Service.