



ODOUR THRESHOLDS

Compilations of odour threshold values
in air, water and other media (Edition 2011)

L.J. van Gemert

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(second enlarged and revised edition)

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PREFACE SECOND EDITION

This edition is revised and enlarged. Errors were corrected and more trivial names included. And a large number of CAS (Chemical Abstract Service) Registry Numbers were added.

Around three thousand new threshold values found in the literature were included in the compilations.

A table with approximate total numbers of compounds, threshold values and references is given below.

<i>Compilation</i>	<i>Compounds</i>	<i>Threshold values</i>	<i>References</i>
AIR	1,790	4,570	740
WATER	1,860	3,840	620
OTHER MEDIA	760	2,340	420
Total		10,750	

L.J. van Gemert, August 2011

INTRODUCTION

General

Many volatile compounds have been identified in food products, as well as in water and air. The importance of these compounds for the odour or aroma of foods and drinks as well as their contribution to odour pollution of air and water can be assessed if their concentrations and odour threshold values are known.

In order to facilitate this assessment already in 1977 compilations were published on odour threshold values in air and water as accurate and exhaustive as possible ⁽¹⁾. In the following years a number of cumulative supplements have been prepared, the last one in 1984 ⁽²⁾. Based on the original compilation, its supplement and some additional data the threshold values in air were standardized and the results of this were published ⁽³⁾.

The present compilations contain almost 8,000 individual threshold values. In total about 1350 references are listed and the number of compounds ranges from approximately 570 for the compilation with odour threshold values in other media, to approximately 1580 for the compilation with odour threshold values in water. The one for air contains threshold values for about 1150 compounds.

Types of odour thresholds

Two types of odour thresholds, i.e. the absolute and the difference threshold, can be distinguished. The detection and the recognition thresholds are absolute thresholds. The first being the minimum concentration which can be detected without any requirements to identify or recognize the stimulus, while the second one is the minimum concentration at which a stimulus can be identified or recognized.

Detection and recognition threshold values are listed and if known, indicated as such. Difference thresholds, the smallest change in concentration of a substance required to give a perceptible change, are not listed.

It is assumed that all threshold values obtained by direct sniffing are based on perception by the sense of smell. But, of course, other modalities, like the common chemical sense, can be involved too.

Definition of threshold value

There are different definitions or calculation methods for the threshold value. These vary from defining the threshold value as the lowest (most sensitive subject) detection threshold to the highest (most insensitive subject) recognition threshold. Standardization based on comparison of these different interpretations has not been applied.

Concentration units

A great diversity of concentration units is used in the literature. For comparison reasons all data have been converted, if necessary, to mg/m³ for odour threshold values in air and to mg/kg for those in water and in other media. Most conversions are straight forward. Due to the differences between the relevant tables, this is not the case with the conversion of threshold values in air reported as dilution factors for the saturated vapour or as vapour pressure values. Threshold values converted in this way, may vary up to 20 % depending on the formula used.

For the conversion of the threshold values in water or other media volume units to weight units the specific weight of the volatile compound or media was not taken into account, i.e. it was supposed to be unity.

Gaschromatography-Olfactometry and odour threshold values in air

In a number of references just the amount injected into the gaschromatograph is reported as threshold value. For conversion into weight per volume units it was assumed that the amount injected was diluted in 100 ml air when smelling.

Media

There are three different compilations in this publication. Those for odour threshold values in air or water have been published before^(1,4). This time also odour threshold values determined in media other than air or water are listed. In this compilation after every threshold value the medium is shortly described.

Original sources

Only data from original references have been compiled, i.e. from publications in which the actual determination of the threshold values is described, or in which the values are given for the first time. Same groups or laboratories report threshold values without reference to the earlier published articles in which the threshold value was reported for the first time. In such cases publications - from the same group - are referred to in which the threshold value is reported.

Nomenclature

In general the rules for the nomenclature from the International Union of Pure and Applied Chemistry (IUPAC) have been followed. A number of trivial names is included with reference to the systematic names. Data for apparent mixtures or for compounds with incomplete names (for instance, chloronitrobenzene without an indication of the position of the substituents) have not been included. An exception was made for mixtures of (*Z*)- and (*E*)-geoisomers, (*R*)- and (*S*)-enantiomers (and diastereoisomers) and cis/trans configuration epimers.

Organization of the compilations

In all three compilations the compounds are listed alphabetically, ignoring structural prefixes. For each compound the data are given chronologically. The references are quoted by author(s) and the year in which the relevant article has been published. Full titles are given in the list of references.

Other compilations

Compilations on taste or flavour thresholds values in water and other media are being prepared at the moment. These compilations will also be available in the future.

Acknowledgements

Many persons have contributed in some way or another to the compilations during the past 30 years. Some were helpful in finding articles with threshold data, others suggested improvements in the nomenclature, including the trivial names, of the chemical compounds and a few had comments on the conversion of the concentration units. All contributions are appreciated very much.

And I am grateful to Pieter Punter of Oliemans Punter & Partners BV, who enabled the publishing of this compilation. The Edition 2003 contains the same threshold data as the first printing⁽⁵⁾.

Your comments are welcomed

A lot of effort and hard work has been put into the compilations in order to make these as accurate and complete as possible. But, it is impossible to exclude errors or to find all available information. Therefore, I would be very grateful if users of these compilations could inform me of any errors or omissions.

Leo van Gemert, Zeist, The Netherlands

IMPORTANT

The threshold data are derived from a search in the literature. By any doubt, the original references should always be consulted.

The threshold values are compiled with the necessary care. It cannot be guaranteed that the data are free of errors. The author and publisher are not liable for damage resulting from the use of the data in these compilations.

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For additional information, please visit our website www.thresholdcompilation.com or send an email to info@thresholdcompilation.com. On our website you can also find information about our compilations of flavour and/or taste thresholds.