PHYSICAL CONSTANTS OF ORGANIC COMPOUNDS

The basic physical constants for over 12,000 organic compounds are presented in this table, along with structures and references to other sources of information. An effort has been made to include the compounds most frequently encountered in the laboratory, the workplace, and the environment. The selection was based mainly on the appearance of the compounds in various specialized tables in this Handbook and in other widely used reference sources, such as the Merck Index and the DIPPR Database of Pure Compound Properties. The occurrence of a compound on regulatory lists of hazardous chemicals was also taken into consideration, as was the availability of reliable physical constant data. Clearly, criteria of this type are somewhat subjective, and compounds considered important by some users have undoubtedly been omitted. Suggestions for additional compounds or other improvements are welcomed.

The data in the table have been taken from many sources, including both compilations and the primary literature. Where conflicts were found, the value deemed most reliable was chosen. Some of the useful compilations of physical property data are listed at the end of this introduction.

In the default listing, the table is arranged alphabetically by the substance name which, in most cases, is either an IUPAC systematic name or, in the case of pesticides and pharmaceuticals, a simple trivial name. Synonyms are given in the column following the primary name. The explanation of the data columns follows:

- **mol. formula**: The molecular formula written in the Hill convention.
- **CAS Registry No.**: The Chemical Abstracts Service Registry Number assigned by CAS as a unique identifier for the compound.
- **Merck No.**: Monograph Number in *The Merck Index, Twelfth Edition*. It should be noted that this is not a unique identifier for a single compound, since several derivatives or isomers of a compound may be included in the same Monograph.
- **Beilstein reference**: Citation to the Beilstein Handbook of Organic Chemistry. An entry of 5-18-11-01234, for example, indicates that the compound may be found in the 5th Series, Volume 18, Subvolume 11, page 1234.
- **mol. weight**: Molecular weight (relative molar mass) as calculated with the 1991 IUPAC Standard Atomic Weights.
- **melting point**: Normal melting point in °C. A value is sometimes followed by [decomposes], indicating decomposition is observed at the stated temperature (so that it is probably not a true melting point).
- **b.p., normal**: Normal boiling point in °C. This is the temperature at which the liquid phase is in equilibrium with the vapor at a pressure of 760 mmHg (101.325 kPa). When a notation such as [decomposes] or [explodes] follow the value, the temperature may not be a true normal boiling point.
- **b.p., low pressure**: The pressure for the boiling point is appended in brackets.
- **density**: Density (mass per unit volume) in g/cm^3. The temperature in °C follows in brackets. Values are given only for the liquid and solid phases, and all values are true densities, not specific gravities. The number of decimal places gives a rough estimate of the accuracy of the value.
- **refractive index**: Refractive index, at the temperature indicated in brackets. Unless otherwise indicated, all values refer to a wavelength of 589 nm (sodium D line). Values are given only for liquids and solids.
- **solubility**: Qualitative indication of solubility in common solvents on a relative scale: 1 = insoluble; 2 = slightly soluble; 3 = soluble; 4 = very soluble; 5 = miscible; 6 = decomposes.

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