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## **Guide to the CRC Handbook of Chemistry and Physics Physical Constants of Organic Compounds (Section 3)**

### **What's in it?**

Physical constants and structure diagrams for nearly 11,000 organic compounds

### **Organization**

Section 3 consists of a tabular arrangement of substances presented alphabetically by the Primary name of the substance. It contains data on Molecular Formula, Molecular Weight, Chemical Abstract Service-Registry Number or CAS-RN, Melting points (mp), Boiling points (bp), Density (den), refractive index (np), Solubility (i= insoluble, sl= slightly soluble, s=soluble, vs=very soluble, msc= miscible, dec= decomposes) and Physical form (liq=liquid, gas, cry=crystal). **See introduction to section 3 for full list of abbreviations.**

### **Before you start**

- Organic compounds are any of a large class of chemical compounds whose molecules contain CARBON.
- Inorganic compounds are chemical compounds NOT containing hydrocarbon groups.
- You have to use the **Hill Order** to search for a chemical compound using its molecular formula. Simply count all the carbons and hydrogens in the molecule and arrange them in the following order: C, H, (and then all other elements arranged alphabetically) (e.g.) ClC6H3(NO2)CF3 is written as C7H3ClF3NO2
- If you already have a CAS registry number check the CAS Registry Number Index, match your CAS number with the appropriate number and locate that number in the far left column in the beginning of Section 3. E.g., if your CAS-RN is 929-73-7 that refers you to number 4642 which in turn shows that your compound is known as Dodecylamine hydrochloride and that among other things has a molecular weight of 221.810 and is very soluble (vs) in water.
- CRC tables rely on abbreviations (e.g., molecular weight=mol. Wt; soluble=s, very soluble=vs). **A complete listing of abbreviations appears on the introductory portions of the tables.**
- Although this handout refers to the CRC's 84<sup>th</sup> edition students can use it to navigate older & newer editions of the CRC. **The CRC is published yearly. You can start your search for physical properties using any year but chances are you may have to use more than one year since some compounds may not appear in every edition.**

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### **How to Search**

To the left of the compound's primary name, you will see a number. This number refers to the second part of Section 3 that shows the chemical structure of the compound listed so you can tell if you have identified the correct compound.

Section 3 also contains a Synonym index. Be mindful that a chemical compound may be listed under several names, so if you are not looking up the compound by its "proper" name you might not find it listed in the handbook. If you cannot find your compound, try the synonym index, which lists alternate names. To the right of the compound, you will see a number, which refers to the number in the far left column in the beginning of Section 3. Section 3 also lists compounds by their

molecular formula or Mol. Form (written in Hill Convention, i.e., Carbons, Hydrogens and all other elements in alphabetical order). For each molecular formula you will see a number and a name. The number will refer you to the beginning of section 3 where all the compounds are listed with their property information.

Next in section 3 you will see an Index of CAS-RN (Chemical Abstract Service Registry Number). If you have found your compound's CAS Registry Number from a different database, you can look it up in this section and you will be directed to the number of where your compound is located.

Finally, in section 3, melting points of various substances are listed in ascending order. If you know that your compound has a melting point of 77 degrees, the index will list several compounds that match these criteria. The number of the compound is listed below, so you can easily look it up in the beginning of section three.

**Sample question:**

Find the molecular weight, boiling point and melting point of 1- Hexanamine. Is this compound soluble in water?

**Step 1:** Find your compound common name because the CRC is organized by the primary name of the substance it makes sense to find out the common name for 1-Hexanamine.

**Step 2:** Start with the synonym index. A glance at the synonym index locates 1-Hexanamine. Next to it is the number 5889. That number refers to the number in the far left column in the beginning of Section 3.

**Step 3:** Return to the CRC's *Physical Constants of Organic Compounds* section. Locate the number 5889 in the far left column in the beginning of Section 3. Now we know that 1-Hexanamine is also known as Hexylamine (its common name). From this table we also learn that its molecular formula (C<sub>6</sub>H<sub>15</sub>N), CAS number (111-26-2), molecular weight (101.90) physical form (liquid), melting (-22.9) and boiling point (132.8) and the fact that it is soluble (sl) in water and miscible (msc) in Ethanol (EtOH) and diethyl ether (eth) and soluble (s) in chloroform (chl).