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# Reliable data sources for key industrial chemicals

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## DATA ITEM No.87009

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The work of the permanent professional staff of the Engineering Sciences Data Unit on this particular Item was monitored and guided by the Physical Data and Reaction Kinetics Committee which has the following constitution:

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The work on this Item was carried out by the Internal Flow and Physical Properties Group of the Engineering Sciences Data Unit. The initial assessment of the available information and the subsequent development of the Item was undertaken by

Mr C.F.Beaton — Independent.

The Physical Data and Reaction Kinetics Committee, which first met in May 1966, has the co-operation of many engineers and scientists in industry, research establishments and universities from whom much assistance and information are being received.

In order to assist the preparation of new work, and particularly to assist the periodic review and revision of work already issued, users are encouraged to make known their experience in using the information and procedures and to notify ESDU of any additional information which they can provide or to which reference can be made. Whenever Items are revised, holders of Volumes automatically receive any material required for up-dating. However, all users are advised to check with ESDU from time to time that Items held are the latest issue and incorporate the latest amendments. Any missing amendments can be supplied on request.

*(Continued on inside back cover)*

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## RELIABLE DATA SOURCES FOR KEY INDUSTRIAL CHEMICALS

## 1. INTRODUCTION

The chemical engineer is constantly requiring physical data for the design of chemical plants, and principally he is concerned with the thermodynamic and transport properties of the materials involved. Databanks will eliminate the need for time-consuming searches, but are often too expensive for the small-scale operator, and will not always meet the requirements of a specialist user needing original data from a known source.

A compilation of reliable data sources for the thermodynamic and transport properties has therefore been prepared for 86 key industrial chemicals. Many of these sources are not widely known in the engineering community and may be difficult to find. Given knowledge of the existence of a text and details of author and publisher, however, they can usually be obtained from scientific libraries such as the British Lending Library in the UK.

Where the property of a particular compound has been researched by ESDU, the number of the particular Data Item is given as the only reference. It should be noted, however, that in a few instances source documents referenced in the Data Item will provide data over a wider range of pressures than are reported in an ESDU Item dealing only with saturation conditions.

Users of ESDU data will appreciate that it is ESDU's objective to provide data by correlation of the experimental data reported in the literature and to extend the extrapolation of results to the highest temperatures consistent with current knowledge of science in this field of study.

Other sources of data listed here are, wherever possible, definitive, or judged to be the best available. Sources more readily available are also included wherever possible. The existence of a source in the following tables, however, indicates only that some data are available; it must not be assumed that all requirements of temperature and pressure are covered.

A few references are made to the loose-leaf data collections of the Thermodynamics Research Center at Texas A & M University. These are a valuable resource, and are usually available at reference libraries; likewise the Tables of Landolt-Bornstein and the literature retrieval guides published by the Cindas Project at Purdue University would almost certainly provide further data and/or sources for many of the chemicals listed.

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## THE TABLES

The tables are arranged in two groups of properties:-

Table I - Thermodynamic Properties

Table II - Transport Properties.

There are five sets of tables for:-

- a) hydrocarbons,
- b) alcohols,
- c) organic oxygen and nitrogen compounds,
- d) halogenated hydrocarbons,
- e) inorganic compounds and solutions.

Each set of compounds is listed in alphabetical order.

In the tables a **five-figure number** is the ESDU Data Item, where available. A **three-figure number** indicates the reference source, with the first two figures giving the date.

Where there is no ESDU Data Item, two references are given wherever possible, the first being the preferred source. Where the number is given in parentheses the source gives an estimated value and/or curve for the property over a wide temperature range.

In the case of vapours the references marked with an asterisk will give the value of the property for the ideal gas.

Where a source is listed under other references it is given as a useful alternative text for any or all other properties of the material.

TABLE Ia  
HYDROCARBONS  
THERMODYNAMIC PROPERTIES

|    | COMPOUND       | VAPOUR<br>PRESSURE | DENSITY |         | HEAT CAPACITY/<br>ENTHALPY |           | LATENT<br>HEAT |
|----|----------------|--------------------|---------|---------|----------------------------|-----------|----------------|
|    |                |                    | LIQUID  | VAPOUR  | LIQUID                     | VAPOUR    |                |
| 1  | ACETYLENE      | 86001              | 561,671 | 561,671 | 561,671                    | 764,561   | 561,671        |
| 2  | BENZENE        | 86012              | 73009   | 73009   | 73009                      | 73009     | 73009          |
| 3  | BUTA-1,3-DIENE | 86001              | 861,751 | 861,751 | 86023                      | 451,751   | 861,751        |
| 4  | BUTANE         | 84022              | 87010   | 823,731 | 86007                      | 823,731   | 823,731        |
| 5  | BUT-1-ENE      | 85008              | 870-671 | 801,671 | 86023                      | 671,870*  | 861,671        |
| 6  | CUMENE         | 86012              | 870,861 | 861     | 75015                      | 764,(766) | 861,751        |
| 7  | CYCLOHEXANE    | 86016              | 870,861 | 861,801 | 764,767                    | 764,870*  | 870,861        |
| 8  | ETHANE         | 84022              | 87010   | 762,731 | 86007                      | 762,731   | 762,731        |
| 9  | ETHYLENE       | 85008              | 811,870 | 811,731 | 86023                      | 811,731   | 811,731        |
| 10 | HEPTANE        | 84022              | 87010   | 801,731 | 86007                      | 731,870*  | 861,731        |
| 11 | HEXANE         | 84022              | 87010   | 801,731 | 86007                      | 731,870*  | 861,731        |
| 12 | ISOBUTANE      | 84022              | 87010   | 824,731 | 86007                      | 824,731   | 824,731        |
| 13 | ISOOCTANE*     | 84028              | 87010   | 861,751 | 86007                      | 870*      | 861,853        |
| 14 | METHANE        | 84022              | 87010   | 763,741 | 86007                      | 763,741   | 763,741        |
| 15 | NAPHTHALENE    | 870,751            | 751     | 751     | 75015                      | 751,870*  | 751            |
| 16 | OCTANE         | 84028              | 87010   | 801,731 | 86007                      | 731,870*  | 861,853        |
| 17 | PENTANE        | 84022              | 87010   | 801,731 | 86007                      | 771,731   | 861,771        |
| 18 | PROPANE        | 84022              | 87010   | 822,731 | 86007                      | 822,731   | 822,861        |
| 19 | PROPYLENE      | 85008              | 802,861 | 802,731 | 86023                      | 802,731   | 802,861        |
| 20 | STYRENE        | 86027              | 861,702 | 861,523 | 75015                      | 764,870*  | 861,751        |
| 21 | TOLUENE        | 86012              | 74024   | 74024   | 74024                      | 74024     | 74024          |
| 22 | XYLENES        | 86012              | 861,870 | 801,861 | 75015                      | 870*      | 861,751        |

\* 2,2,4-Trimethylpentane

TABLE IIa  
HYDROCARBONS  
TRANSPORT PROPERTIES

| COMPOUND       | VISCOSITY |             | THERMAL CONDUCTIVITY |             | SURFACE TENSION | OTHER REFS. |    |
|----------------|-----------|-------------|----------------------|-------------|-----------------|-------------|----|
|                | LIQUID    | VAPOUR      | LIQUID               | VAPOUR      |                 |             |    |
| ACETYLENE      | 662,(705) | 752,751     | (705)                | 703,662     | 724             | 714         | 1  |
| BENZENE        | 81016     | 752,751     | 84010                | 703,751     | 724             | 671         | 2  |
| BUTA-1,3-DIENE | 751,(766) | (766)       | 75009                | (766)       | (766)           | -           | 3  |
| BUTANE         | 79027     | 752,751     | 75003                | 703,751     | 724             | 765         | 4  |
| BUT-1-ENE      | 80015     | 751,(766)   | 75009                | 782,(766)   | 724             | 714         | 5  |
| CUMENE         | 81016     | (766),(705) | 84010                | (766),(705) | 724             | -           | 6  |
| CYCLOHEXANE    | 751,870   | 751,(622*)  | 77010                | 831,782     | 724             | -           | 7  |
| ETHANE         | 79027     | 773,752     | 75003                | 773,703     | 724             | 751         | 8  |
| ETHYLENE       | 80015     | 752,726     | 75009                | 703,726     | 724             | 765         | 9  |
| HEPTANE        | 79027     | 752,751     | 75003                | 703,751     | 724             | -           | 10 |
| HEXANE         | 79027     | 752,751     | 75003                | 703,751     | 724             | -           | 11 |
| ISOBUTANE      | 79027     | 752,751     | 75003                | 703,765     | 724             | -           | 12 |
| ISOOCTANE      | (705)     | (705)       | 75003                | (705)       | (705)           | -           | 13 |
| METHANE        | 79027     | 704,752     | 75003                | 703,704     | 724             | 722         | 14 |
| NAPHTHALENE    | 81016     | (766)       | 84010                | (766)       | 724             | 772         | 15 |
| OCTANE         | 79027     | 752,751     | 75003                | 703,751     | 724             | -           | 16 |
| PENTANE        | 79027     | 752,751     | 75003                | 703,751     | 724             | 691         | 17 |
| PROPANE        | 79027     | 793,752     | 75003                | 793,703     | 724             | 751         | 18 |
| PROPYLENE      | 80015     | 752,726     | 75009                | 703,726     | 724             | 765         | 19 |
| STYRENE        | 81016     | (766),(705) | 84010                | (766),(705) | 724             | 792         | 20 |
| TOLUENE        | 81016     | 80017       | 84010                | 703,782     | 724             | 705         | 21 |
| XYLENES        | 81016     | (766),(705) | 84010                | (766),(705) | 724             | -           | 22 |

TABLE 1b  
ALCOHOLS  
THERMODYNAMIC PROPERTIES

|    | COMPOUND    | VAPOUR<br>PRESSURE | DENSITY |         | HEAT CAPACITY/<br>ENTHALPY |           | LATENT<br>HEAT |
|----|-------------|--------------------|---------|---------|----------------------------|-----------|----------------|
|    |             |                    | LIQUID  | VAPOUR  | LIQUID                     | VAPOUR    |                |
| 23 | BUTAN-1-OL  | 74023              | 861,501 | 861,801 | 79028                      | 623,870*  | 861,853        |
| 24 | CRESOLS     | 81025              | 82032   | 82032   | 82032                      | 82032     | 82032          |
| 25 | ETHANEDIOL  | 861,870            | 861,501 | 861     | 852,794                    | (705*)    | 861,(521)      |
| 26 | ETHANOL     | 74023              | 861,751 | 861,751 | 79028                      | 751,870*  | 861,853        |
| 27 | GLYCEROL    | 861,751            | 861,751 | 861     | 852,751                    | 681(705*) | 861,681        |
| 28 | METHANOL    | 74023              | 80017   | 80017   | 79028                      | 775,870*  | 80017          |
| 29 | PHENOL      | 81025              | 82004   | 82004   | 82004                      | 82004     | 82004          |
| 30 | PROPAN-1-OL | 74023              | 861,501 | 861,501 | 79028                      | 623,870*  | 861,853        |
| 31 | PROPAN-2-OL | 74023              | 76012   | 76012   | 79028                      | 76012     | 76012          |
| 32 | XYLENOLS    | 81025              | 83005   | 83005   | 83005                      | 83005     | 83005          |

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