DETHERM Thermophysical database at the Physical Sciences Data-science Service

What is **DETHERM**?

DETHERM is one of the largest thermophysical databases in the world containing:

- 11,300,000 data sets
- 163,000 mixtures
- 60,600 pure compounds

What sort of data is present?

The data present in DETHERM is broadly classed as thermophysical:

Phase equilibrium (activity coefficients, gas solubilities)

Azeotropic data

Excess properties (enthalpies, heat capacities, volumes)

Pure component properties

Caloric and acoustic properties

Electrochemical properties

Pressure-Volume-Temperature (PVT) properties

Transport properties

Surface properties

Thermal conductivities

Viscosities

Solubilities

Diffusion Coefficients

Eutectical Data

Access DETHERM via the

Physical Sciences Data-science Service

at www.psds.ac.uk

email: info@psds.ac.uk

DETHERM

How can I search DETHERM?

DETHERM allows the searching of **pure substances** and **mixtures**.

Search for components and define a mixture:

Name	(e.g. ethanol)
Sum formula	(e.g. C2H6*)
CAS-Nr	(e.g. 64-17-5)

Search

Clear

- Enter a Name or a Sum Formula or a CAS-Nr to search for substances.
- You can use the * wildcard with names and sum formulae.
- Enter a Name and a Sum Formula string to search for substances that should match both criteria.
- A field accepts multiple search strings separated by a ;.

Where does the data come from?

The complete DETHERM database consists of **externally maintained packages**:

Electrolyte Data Collection (ELDAR)

Thermophysical Database (**INFOTHERM**) Data Collecti

Data Collection (**C-DATA**)

Dortmund Data Bank (**DDB**)

Thermophysical Parameter Database (**COMDOR**) Solubility Database (**CAPEC-SDB**)

How do I access DETHERM?

DETHERM is provided to the UK academic community via the **PSDS at** <u>www.psds.ac.uk</u>. DETHERM has been developed by DECHEMA e.V. The Physical Sciences Data-science Service is funded by the EPSRC.

Access is authenticated by UK academic IP address via **<u>www.psds.ac.uk</u>**. For offcampus working, a PSDS username / password will be issued.

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