DETHERM Thermophysical database at the Chemical Database Service

What is DETHERM?

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

- 4,200,000 data sets
- 129,500 mixtures
- 38,850 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

Chemical Database Service at <u>detherm.cds.rsc.org</u>

email: <u>cds@rsc.org</u>

DETHERM

Thermophysical database

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**)

Dortmund Data Bank (**DDB**)

M) Data Collection (**C-DATA**)

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

How do I access DETHERM?

DETHERM is provided to the UK academic community via the **Royal Society of Chemistry-hosted Chemical Database Service** at <u>cds.rsc.org</u>. DETHERM has been developed by DECHEMA e.V. The Chemical Database Service is funded by the EPSRC.

Access is authenticated by UK academic IP address via **<u>detherm.cds.rsc.org</u>**. For offcampus working, a Chemical Database Service username / password will be issued.

Access DETHERM via the Chemical Database Service at <u>detherm.cds.rsc.org</u>

email: cds@rsc.org