STN®

THE CHOICE OF PATENT EXPERTS™

ReaxysFile on STN

Introduction and Property Glossary

1. Introduction

ReaxysFile is a factual database. Covering historical data back to 1771 and the most important current journals and patents within chemistry.

For indexed substances, ReaxysFile offers comprehensive information including pharmacological and ecological data as well as chemical data and physical properties. Storage of this information in many different topics enables precise retrieval for specific information.

2. Content

ReaxysFile covers the whole spectrum of organic and inorganic chemistry. All important chemistry-related disciplines are covered:

- Synthetic chemistry

Experimental reaction and substance data – from organic, inorganic and organometallic chemistry

- Medicinal chemistry, biochemistry and life sciences

Structure-activity-relationship data

- Analytical and physical chemistry

Validated spectral data such as NMR shifts and additional physical property data

- Environmental chemistry

Information such as toxicant uptake in biological systems

- Materials chemistry
  - Coordination compounds and catalysts, e.g. in polymer research
  - Alloys, glasses and ceramics
  - Factual data e.g. on semi-and superconductivity, magnetism, optical and mechanical properties

- REACH data

3. Substance Types

ReaxysFile has extended the concept of substances to enable the abstraction of environmental, pharmacological and toxicological and patent data. It now allows the acceptance of substances whose identity is not necessarily given by means of a structure.
ReaxysFile distinguishes between several types of substances:

3.1. Pure substances with a structural formula

Substances of this type may consist of one (e.g. benzene) or more fragments (e.g. salts, complexes, addition compounds, each with defined molar ratios).
Peptides with up to 12 amino acids and polysaccharides with up to 6 carbohydrate units are abstracted. Larger peptides and polysaccharides are registered by means of their names as biomolecules.

3.2. Substances which may be described by means of names or information about the components

- Biomolecules (biopolymers, carbohydrates, nucleic acids, proteins, enzymes, hormones, etc.)
- Mixtures (composed of components)
- composition completely given
- composition partially given
- composition completely not given
- Polymers
- monomers given
- monomers not given
- Solid Solution

3.2.1. Mixtures

Mixtures are only abstracted when it is clear from the publication that the substance or its components belong to the area of organic chemistry. Frequently they are chemical products which are commercially available as pesticide or a cleaning material. The active components are then usually known but various additives in various concentrations are used by different manufacturers. This substance type is divided into different substance types.

- Mixtures (Composition completely given)
  "Composition known" means that not only the components (names or structures) but also their concentrations in the mixture are known completely and exactly (author's values). The mixtures name would not need to be known.

- Mixtures (Composition partially given)
"Composition partly known" mean that the qualitative and/or quantitative composition (components, concentrations) are not completely known. Alternatively all data are available but for the concentrations only ranges are given. The mixture is described by means of its name.
- Mixtures (Composition completely not given)
"Composition unknown" means that there are no data available for the components nor their concentrations. Only the name of the mixture is given (and the certainty that a mixture is being dealt with). The mixture is completely described by its name.

3.2.2. Polymers

Included are the synthetic polymers. This substance type is divided into two substance types.

- Polymers (Monomers given)

Polymers of this type are described by the name of the polymer and the structure of the monomers (structure entry for the components). The names of the polymers are entered with a strict syntax.

- Polymers (Monomers not given)

This type of substance is completely described by its name only.

3.3. Inorganic Substances

- Alloys
- Glass or ceramic material
- Minerals

3.4. Coordination Compounds

A class of substances with chemical structures in which a central metal atom is surrounded by nonmetal atoms or groups of atoms, called ligands, joined to it by chemical bonds. Coordination compounds include such substances as vitamin B12, hemoglobin, and chlorophyll, dyes and pigments, and catalysts used in preparing organic substances.

4. Single-Component Systems

Available properties:

- Structure and Energy Parameters (SEP)
- Physical State (SAG) including Crystal Data
- Transport Phenomena (TRA)
- Thermochemical Data (THE)
- Optical Properties (OPTP)
- Spectra (SPE)
- Magnetic Properties (MAGP)
- Electrical Properties (ELEP)
- Electrochemical Behaviour (ECB)
- Safety Data (SF)
- Further Information (FINFO)

5. Multi-Component Systems (MCS)

Available properties:

- Liquid/Liquid Systems (MCS) (LLSM)
- Liquid/Solid Systems (MCS) (LSSM)
- Mechanical & Physical Properties (MCS) (MECM)
- Transport Phenomena (MCS) (TRAM)
- Energy Data (MCS) (ENEM)
- Electrical Data (EDM)
- Optical Data (ODM)
- Boundary Surface Phenomena (MCS) (BSPM)
- Adsorption (MCS) (ADSM)
- Association (MCS) (ASSM)

6. Property Parameter Fields

This data fields contains the parameter dependency of physical properties as temperature and pressure.

7. Proximities for Searching Property Information

In physical data searches the (P) paragraph operator will be used frequently. This operator links terms within the same subfield: e.g. the enthalpy of formation to a given temperature and to a given pressure, not to some other temperatures or pressures in the same record.

Following operators are allowed in a descending order of execution:

1. all numeric operators
2. (W), (nW), (A), (nA)
3. (S)
4. (P)
5. (L)
6. AND, NOT
7. OR

8. Units Conversion

The unit systems available in the ReaxysFile are: SI, MKS, CGS, STN (commonly used metric units), FPS, and ENG (commonly used U.S. Engineering units)

9. Bibliographic Search

ReaxysFile contains citations from Journals, Patents and books or monographs. Titles of journals with CODEN will be found in /JT field, for journals and other works without CODEN the title is stored in /JTW field.

The references are automatically displayed with the corresponding property.

Bibliographic Information consists of the following topics and fields:

- All Journal Titles /AJT
- Author /AU
- CODEN /ISN
- Document Type /DT
- Journal Title /JT
- Journal Review without CODEN /JTW
- Language Code /LA
- Patent Assignee /PA
- Patent Country /PC
- Patent Number /PN
- Publication Year /PY
- Citation (unresolved) /URES

(URES: Citations that could not be classified into /JT or /JTW, e.g. Tech. Note Nr. 1019 (1946).

10. Structure Search

Types and Scopes of Structure Searching

Search type: All types have the same definitions as they have in the other structure-searchable files on STN.

- Substructure (SSS)
- Closed Substructure (CSS)
- Exact (EXA)
- Family (FAM)

Search scope: All scopes have the same definitions as they have in the other structure-searchable files on STN. They determine how much of the file is searched.

SAMPLE (SAM)	Representative portion of the file (default)
FULL (FUL)	100% of the file
RANGE (RANGE)	User-specified portion of the file
SUBSET (SUB)	User-defined set of the file

11. DISPLAY Formats

ALL displays all information available about a record. Use this format with caution. Records are often quite lengthy.

QRD (Query Related Display) is the display default format if no format is specified: IDE plus HIT.

IDE (Identification of Substance) is the display format including all substance identifying information and Field Availability. Hit term highlighting is available for this format.

Further, predefined formats are available (for a detailed list of included fields see Summary Sheet).

12. REACH Relevant Data

The predefined format may contain the following properties

- Melting Point (MP)
- Sublimation Point (SP)
- Boiling Point (BP)
- Vapour Pressure (VP)
- Optical Rotatory Power (ORP)
- Refractive Index (RI)
- Mutarotation (MUT)
- Density (liquid) (DEN)
- Dissociation Exponent (DE)
- Solubility (SLB)
- Heat Capacity(CP)
- Heat capacity (CV)
- Enthalpy of Formation (HFOR)
- Enthalpy of Vaporization (HVAP)
- Ecological Data (ECO)
- Pharmacological Data (PHARM)
- Flash Point (FP)

13. Glossary (alphabetical order) of Properties

Abiotic Degradation, Photolysis (ECDP)

The property describes the degradation process via photochemical reactions such as photooxidation, photomineralisation without the participation of organisms.

Accession Number (AN)

The ReaxysFile Accession Number is the number of the substance record in the ReaxysFile. It is an integer, which does not contain further information.

Acoustic Properties (SOUND)

This field contains information about

- Velocity of sound
- Sound absorption
- Acoustic relaxation
- Ultrasonic properties
- Ultrasonic velocity
- Hypersonic velocity
- Ultrasonic absorption
- Hypersonic absorption

Adsorption MCS (ADSM)

The field Adsorption Description (/ADSM.KW) contains keywords from the following list of controlled terms:

- Adsorption
- Adsorption isotherm
- Chemisorption
- Enthalpy of adsorption
- Further physical properties of the adsorbed molecule
- Desorption
- Adsorption and desorption isotherms
- Rate of adsorption
- Desorption isotherm(s)
- Rate of desorption

Association MCS (ASSM)

The field Association Description (/ASSM.KW) contains keywords from the following list of controlled terms:

- Association with compound
- Stability constant of the complex with ...
- Enthalpy of association
- Dipole moment of the complex
- Spectrum of the complex
- Further physical properties of the complex
- Exciplex formation
- IR spectrum of the complex
- NMR spectrum of the complex
- UV/VIS spectrum of the complex

Basic Preferred Registry Number (BPR)

The Basic Preferred RN is the single CAS Registry Number that has been selected as the best choice for a compound from the one or more RNs that may be present in the database. The BPR is, however, not always present and is selected according to the following criteria:

1. If there is only one RN available from all sources, this will also be BPR.
2. Some compounds have one or more Registry Numbers that have been assigned by CAS. If ReaxysFile has one of these Registry Numbers on record in its file, this RN will be the BPR. If, however, ReaxysFile has different Registry Numbers in its file, the compound will not be given a BPR and only the CAS supplied numbers will appear in the RN field.
3. If a compound has several RNs in its file, these RNs will appear in the compound record, but no BPR will be given.

Biological Behavior (BIO)

This property contains bioaccumulation, bio magnification and bio monitoring data. Bioaccumulation is the ability of organisms to concentrate substances within themselves. Bioaccumulation is the result to two processes: accumulation and elimination. Bio magnification is a sequence of processes in an ecosystem by which higher concentrations of chemical substances are attained in organisms at higher trophic level in the food chain. Bio monitoring has the objective that the appearance of substances is comprehensively monitored.

Biological Behavior (BIO)

This property contains bioaccumulation, biomagnification and biomonitoring data.

Bioaccumulation is the ability of organisms to concentrate substances within themselves. The bioaccumulation is a result of two processes: accumulation and elimination, whereby the rate of intake exceeds the organism's ability to remove the substance from the body. A characteristic measure is the Bioconcentration Factor.

Biomagnification is a sequence of processes in an ecosystem by which higher concentrations of chemical substances are attained in organisms at higher trophic level in the food chain (plants, herbivores, carnivores).

Biomonitoring has the objective that the appearance of substances (and their damaging influences) is comprehensively monitored. This is achieved by the use of bioindicators (birds, fish, lichens, etc.) or biomarkers (CYP1A induction, metallothioneine, DNA-adducts, etc.)

Bioaccumulation data are stored in several fields.

Boiling Point (BP)

The boiling point is the temperature at which the vapor pressure of a liquid equals the external pressure. The normal boiling point is the temperature at which the vapor pressure equals the normal atmospheric pressure.

Bulk Viscosity (BV)

Bulk viscosity is the force per unit area required to maintain unit difference of velocity between two layers 1 cm apart. The values are given at the measurement temperatures and can be searched using the associated parameter field code BV.T.

CAS Registry Number (RN)

The CAS Registry Number search field contains the CAS Registry Number of the ReaxysFile substance. CAS Registry Numbers are not available for all ReaxysFile Substances.

Chemical Name (CN), Chemical Name Segment (CNS), Autonom Name (AUN)

The field Chemical Name contains complete chemical names from various sources:

- the preferred name (the IUPAC based name used in the ReaxysFile Handbook)
- names from the original publication
- names generated by the program AutoNom
- Additionally, compounds can have multiple entries for chemical names such as systematic, trivial and tradenames.

Because the complete chemical name is known comparatively infrequent, Chemical Name Segments (/CNS, search field only) are available for searching. /CNS contains basic and natural segments of a chemical name. To create the natural segments, parentheses and/or brackets, locants and punctuation are removed.

Circular Dichroism (CDIC)

Optically active compounds absorb left and right polarized light unequally. When linearly polarized incident light passing through a substance becomes elliptically polarized the phenomenon is known as circular dichroism. The wavelength range over which this phenomenon has been measured is stored in the CDIC field.

Complex Phase Equilibria (CPEM)

This field contains information about

- Solid-vapor phase equilibrium
- Liquid-solid-vapor phase diagram
- Liquid-solid-vapor phase equilibrium
- Triple point
- Quadruple point
- Phase equilibrium

Compressibility (CMP)

This field contains information about

- Adiabatic compressibility
- Isothermal compressibility

Concentration in Environment (COEV)

gives information on the degree of pollution by hazardous chemicals in living organisms or non-living environmental compartments

Conformation (CNF)

This field contains information about

- Energy barrier
- Energy difference between conformers
- Equilibrium constant
- Equilibrium data
- Kinetics

Critical Density (CRD)

The Critical Density field contains the numerical value for the density of a substance measured at its critical temperature and pressure.

Critical Micelle Concentration MCS (CMC)

The critical micelle concentration is the concentration at which micelles begin to form in a system comprising solvent(s), surfactant(s), possibly other solutes and a defined physical environment. You can search for the associated temperature and solvent information in the parameter fields CMC.T and CMC.SOL.

Critical Pressure (CRP)

The critical pressure is the minimum pressure required liquefying a gas at its critical temperature. The Critical Pressure field contains the value of the critical pressure for the substance.

Critical Temperature (CRT)

The critical temperature is the temperature above which a gas cannot be liquefied by pressure. The Critical Temperature field contains the values of the critical temperature for the substance.

Critical Volume (CRV)

The Critical Volume field contains values for the molar volumes of substances measured at their critical pressures and critical temperatures

Cross Reference (XREF)

The Crossfile Reference contains mostly the chemical name (/XREF.CN) of the compound which is used in the referenced database, the name (/OS) of the referenced database, the document number (XREF.ID) in the referenced database, the datatype (/XREF.DTP) and the corresponding bibliographic references.

Cross-Section (XS)

This field contains information about:

- Photoionization cross-section
- Electron ionization cross-section
- Proton ionization cross-section
- Ionization cross-section
- Collision cross-section

Crystal Phase (CRYPH)

This field contains information about

- Rate of crystallization
- Polymorphism
- Rate of transition
- Crystal habit
- Crystal growth
- Crystal morphology
- Crystal structure determination (crystal lattice parameters)
- Interplanar spacing
- Association in the solid state
- Solid state structure properties
- Melting pressure
- Freezing point
- Glass transition temperature
- Phase diagram
- Long spacing
- Reorientation in the solid state
- Spin polarization
- Nuclear spin conversion
- Structure of the solid
- Dimensions of the unit cell

Crystal Property Description (CPD)

The Crystal Property Description field contains terms that give a qualitative Description of the outward appearance of crystalline materials such as the color of the crystal and its shape.

Crystal Space Group (CSG)

The Space Group field contains information on the different crystal space groups using the relevant terms.

Crystal System (CSYS)

The Crystal System field contains information on the seven crystal classes cubic, hexagonal, trigonal, tetragonal, monoclinic, triclinic and rhombic. You can search in the Crystal System field using the class name of the crystal system of interest.

Decomposition Point (DP)

The decomposition point is the temperature at which a substance undergoes thermal decomposition at atmospheric pressure.

Degradation (ECDH, ECDP, ECS, BIOD)

contains the subdivisions Biodegradation, Abiotic Degradation and Stability in Soil. Biodegradation describes the degradation of an organic substance to smaller molecules or to inorganic substances by microorganisms. This can occur by means of aerobic or anaerobic degradation. The property Stability in Soil characterizes the resistance or stability of a substance in soil. Standardized soils are often used for measurement of specific dissipation times.

Density of Crystal (CDEN)

The field contains the numerical value of the density of the substance in the crystalline state at a particular temperature and pressure.

Density of Liquid (DEN)

Density is defined as mass per unit volume at a particular temperature and pressure. The Density field contains values for the crystal density at 1 atm or below and liquid density at 1 atm when below normal boiling point, at saturation pressure at and above normal boiling point. Because the density varies with the temperature, you can search for the associated measurement temperature and reference temperature in the parameter fields DEN.T and DEN.RT.

Derivative (CDER)

Characterization derivatives and addition compounds (salts, complexes, adducts, associations, clathrates) are recorded as individual compounds with all their data if they fulfill the criteria for the acceptance of a compound given above. In other cases, the Derivative field CDER contains chemical names and additional information about derivatives of the cited substance (e.g. salt names, salt molecular formulae, and melting point of derivatives). The ReaxysFile Accession Number of the derivative can be searched in the parameter field CDER.AN.

Examples for substances used for characterization:

- Picrates
- Phenylhydrazones
- Semicarbazones
- Methohalides
- Acetyl derivatives
- Benzoyl derivatives
- Oximes

Dielectric Constant (DIC)

The dielectric constant is the ratio of the capacity of a condenser with that substance as the dielectric medium to the capacity of the same condenser in a vacuum. The values of the constant are given at specified temperatures and frequencies. You can search for the associated frequency and temperature in the parameter fields DIC.F and DIC.T.

Dielectric Static Constant (DICS)

For a given substance the static dielectric constant is the ratio of the capacity of a condenser with that substance as the dielectric medium to the capacity of the same condenser with a vacuum as the dielectric medium.

The dielectric constant is a function of temperature and frequency at which the alternating electric field varies.

The static dielectric constant is the dielectric constant at frequencies low enough that the equilibrium is maintained as the electric field varies The values of the constant are given at specified temperatures. You can search for the associated temperature in the parameter fields SDIC.T.

Dipole Moment (DM)

This field contains information about

- Bond moment
- Dipole moment
- Quadrupole moment
- Hexadecapole moment
- Octopole moment

Dissociation Exponent (DE)

The dissociation exponent is defined as the logarithm (base 10) of the reciprocal of the equilibrium constant. The Dissociation Exponent field contains the values for the dissociation exponents (pKa for acids, pKb for bases). You can search for the associated information about dissociation group, temperature, solvent, method and type using the parameter field codes DE.GRP, DE.T, DE.SOL, DE.MET and DE.TYP.

Dynamic Viscosity (DV)

Dynamic viscosity is the ratio of the shearing stress to the rate of shear. The Dynamic Viscosity field contains the values for the dynamic viscosity of substances given at specified temperatures. You can search for this associated information using the parameter field code DV.T.

Ecological Data (ECO)

are concerned with effects and interactions of chemical substances, especially environmental chemicals, with living and non-living nature. Their behavior in the environment for instance, their distribution, accumulation potentials and transformation are also focal points of research in ecological chemistry.

Ecological Mobility (ECTD)

This property describes the transport and distribution of chemical substances, especially environmental chemicals, in the non-living environment (air, soil, water) by way of physical processes like absorption, desorption, dispersion, etc.

Ecotoxicology (ECTOX)

is a subdivision of toxicology. It concentrates on the toxic effects of chemical substances on organisms, which are indicators for the degree of polluation in an ecosystem (air, soil, water).Typical species are fish and daphnia for water, earthworms for soil and birds for air. Its aim is to reveal structural and functional changes in the ecosystem due to effects of chemical substances.

Electrical data (ELE)

This field contains information about

- Angle of dielectric loss
- Critical frequency (or wavelength)
- Dielectric anisotropy
- Dielectric increment
- Dielectric loss
- Dielectric relaxation time
- Dielectric saturation
- Relaxation frequency
- Cole-Cole diagram
- Piezoelectricity
- Thermoelectricity
- Photoelectricity (Becquerel effect)
- Electrical conductivity
- Photoconductivity
- Dielectric strength
- Electrical properties
- Photovoltaic effect

Electrical Data MCS (ELE)

This field contains information about:

- Angle of dielectric loss
- Critical frequency (or wavelength)
- Dielectric anisotropy
- Dielectric increment
- Dielectric loss
- Dielectric relaxation time
- Dielectric saturation
- Relaxation frequency
- Cole-Cole diagram
- Piezoelectricity
- Thermoelectricity
- Photoelectricity (Becquerel effect)
- Electrical conductivity
- Photoconductivity
- Dielectric strength
- Electrical properties
- Photovoltaic effect

Electrical Polarizability (POL)

This fields contains information about the following topics

- Atom polarization
- Electron polarization
- Hyperpolarizability
- Molar polarization
- Optical anisotropy
- Polarizability

Electrochemical Behavior (ELCB)

This topic contains information about:

- Autoprotolysis
- Enthalpy of dissociation (electrolytic)/protonation
- Kinetics of dissociation (electrolytic)/protonation
- Enthalpy of neutralization
- Proton affinity
- Electrolytic dissociation/protonation equilibrium
- Thermodynamic parameters for autoprotolysis
- Thermodynamic parameters for dissociation/ protonation
- Volume change on dissociation
- Enthalpy of deprotonation
- Acidity
- Basicity
- Protonation
- Deprotonation
- pK(R+)
- pH of aqueous solutions
- Stability constant
- Electrochemical properties
- Polarography
- Degree of dissociation

Electrochemical Cell (ELCH)

The electrochemical cell potential field contains the values for cells using substances of the file as electrode material, as electrolyte or as compound of the electrolyte. The electrochemical cell potential field is a numeric range searchable field and is linked to the associated temperature. A pair of electrodes dipping into an ionic medium called electrolyte (solid, liquid or gas) and connected by an external electric conductor constitutes an electrochemical cell.

Electrochemical Characteristics (POT)

The field Electrochemical Characteristics Description (/POT.KW) contains keywords from the following list of controlled terms:

- Cyclic voltammetry
- Oxidation potential
- Polarographic current/voltage curve
- Polarographic half-wave potential
- Redox potential
- Reduction potential
- Voltammetry
- Photo-electrochemical half-wave potential

Electrolytic Conductivity (ELYC)

The molar (specific) electrolytic conductivity is the reciprocal of the resistivity, per mole (gram) per unit volume of solution.

The equivalent electrolytic conductivity is the molar electrolytic conductivity per number of equivalents.

Electron Binding (CIP)

This field contains information about

- Electron affinity
- Core IP

Energy Barrier of Conformation (EBC)

The Energy Barrier field contains the values for the amount of energy required to convert one conformation of a molecule to another where both conformations represent energy minima. Conformations are defined as spatial arrangements of the atoms in a molecule, which can be interconverted by rotation about a single bond. You can search for the associated information about the bond type using the parameter field code EBC.TYP.

Energy Data MCS (ENEM)

The field Energy Data Description (/ENEM.KW) contains keywords from the following list of controlled terms:

- Enthalpy of solution
- Enthalpy of mixing
- Enthalpy of dilution
- Enthalpy of evaporation
- Heat capacity of mixtures
- Enthalpy of mixtures
- Entropy of mixtures
- Excess thermochemical parameter
- Thermodynamic properties of system with
- Partial molar enthalpy of mixing
- Heat capacity Cp
- Heat capacity Cv
- Excess heat capacity Cp
- Molar excess Gibbs free energy

Energy of Dissociation (EDIS)

The dissociation energy is defined as the energy required to break a specific bond in one mol of a compound to produce two fragments. You can search for the associated information about the bond type using the parameter field code EDIS.TYP.

Enthalpy of Combustion (HCOM)

The enthalpy of combustion is the change in enthalpy, which occurs when one mol of a compound reacts completely with an excess of oxygen at atmospheric pressure and at room temperature, the products being in their natural physical state under these conditions. The values are given at specified temperatures and pressures. You can search for this associated information using the parameter field codes HCOM.T and HCOM.P.

Enthalpy of Formation (HFOR)

The enthalpy of formation is the change in enthalpy, which occurs when one mol of the compound is formed from its elements each being in its natural state at ordinary temperature and pressure. The values are given at specific temperatures and pressures and can be searched using the parameter field codes HFOR.T and HFOR.P.

Enthalpy of Fusion (HFUS)

The enthalpy of fusion is the change in enthalpy, which occurs when one mol of solid is converted to a liquid at a constant temperature.

Enthalpy of Hydrogenation (HHDG)

Enthalpy of hydrogenation is defined as the change in enthalpy, which occurs when one mol of an unsaturated compound reacts with an excess of hydrogen to become fully saturated at atmospheric pressure and room temperature the reactants and products being in their natural states under these conditions. The values are given at specified temperatures. This field may be linked to associated chemical name or AN of the saturated compound. You can search for this associated information using the parameter field codes HHDG.AN, HHDG.CN and HHDG.T.

Enthalpy of Sublimation (HSUB)

Sublimation is defined as the direct conversion of a solid into a gas at constant temperature and pressure. The enthalpy of sublimation is the change in enthalpy, which occurs when one mol of a substance sublimes at a specified temperature and pressure. The values for this field are given at the sublimation temperature.

Enthalpy of Vaporization (HVAP)

The enthalpy of vaporization is the enthalpy change, which occurs when one mol of a liquid is converted to a vapor at a constant temperature. The values in this search field are cited at specified temperatures and pressures. You can search for this associated information using the parameter field codes HVP.T and HVP.P. If a temperature range has been given in the literature, the average value has been stored.

ESR Data (ESR)

The field ESR Description (ESR.KW) contains keywords from a list of controlled terms:

- Spectrum
- Signals
- ENDOR (electron-nuclear double resonance)
- g-factor
- ESR linewidth
- ESR second moment
- Electron spin-lattice relaxation time
- Electron spin-spin relaxation time
- 1H-electron Overhauser effect
- CIDEP (chemically induced dynamic electron polarization)

- ELDOR (electron-electron double resonance)
- ESR
- ESR-hyperfine coupling constants
- Triplet state ESR spectrum
- Triplet state ESR
- Triplet state ESR g-factor
- Triplet state ESR hyperfine coupling constant(s)
- Triplet state ESR zero-field splitting parameter(s)

Exposure Assessment (EXCA)

describes the spread of pollution originating from natural or synthetic substances or sources, e.g. the contamination of hen feed with dioxins and PCBs due to careless handling.

Field Availability (FA)

The field availability search field indicates if a searched property is available for a given substance or not.

Flash Point (FP)

This is the lowest temperature of the liquid at which it gives off enough vapor to form an ignitable mixture of vapor and air immediately above the liquid surface. A liquid is classified as flammable or combustible depending on its flash point. A flammable liquid has a flash point below 37.8 C while a combustible liquid has a flash point greater than 37.8 C.

Fluorescence (FLU)

The field Phosphorescence Description (PHO.KW) contains keywords from a list of controlled terms:

- Spectrum
- Maxima
- Phosphorescence lifetime
- Phosphorescence decay kinetics
- Phosphorescence quenching
- Degree of polarization of phosphorescence
- Excimer phosphorescence
- Delayed phosphorescence
- Triplet state energy
- Triplet state quantum yield
- Triplet state lifetime
- Triplet state decay kinetics
- Triplet state quenching
- Triplet state sublevel studies
- Energy transfer from triplet state
- Phosphorescence excitation spectrum
- Phosphorescence quantum yield
- Phosphorescence

Further Information (FINFO)

This field contains references for rarely reported physical and chemical properties.

Examples are

- Behavior as catalyst
- Behavior as inhibitor
- Colloid chemical behavior
- Ecological data
- Health protection
- Occurrence in nature
- Polymerization
- Reaction of compound surface
- Reaction with substance classes
- Solvation / hydration

Gas Phase (GP)

This field contains information about:

- Fugacity
- Rotational correlation function of the gas
- Neutron scattering of the gas
- Association in the gas phase

Heat Capacity Cp (CP)

The molar heat capacity at constant pressure is defined as the quantity of heat necessary to raise the temperature of 1 mol of the substance 1 degree at constant pressure. The Values are given at specified temperatures. The Heat Capacity CP field contains calorimetric determined values (see also Cpo). You can search for the associated information about the temperature using the parameter field code CP.T.

Heat Capacity Cpo (CPo)

The molar heat capacity CPo is defined as the quantity of heat necessary to raise the temperature of 1 mol of the ideal gas 1 degree at constant pressure. The Heat Capacity CPo field contains values for ideal gases obtained from statistical thermodynamic calculations (see also CP). You can search for the associated information about the temperature using the parameter field code CPo.T.

Heat Capacity Cv (CV)

The molar heat capacity CV is defined as the quantity of heat necessary to raise the temperature of 1 mol of the substance 1 degree at constant volume. You can search for the associated information about the temperature using the parameter field code CV.T.

Henry Constant MCS (HNC)

The Henry constant is the ratio of the concentration of a chemical substance in air to the concentration in an aqueous solution at equilibrium. It can be used as a qualitative measure about the volatility of the substance and its whereabouts in nature. You can search for the value of the constant or its decadic logarithm. Information on the related temperature and solvent is given in the parameter fields /HNC.T and /HNC.SOL.

InChI Key/ Alternate InChI Key (INCHI, AINCHI)

is a textual identifier for chemical substances. The identifiers describe chemical substances in terms of layers of information – the atoms and their bond connectivity, tautomeric information, isotope information, stereochemistry, and electronic charge information.

Infrared Spectrum (IR)

The field IR Description (IR.KW) contains keywords from a list of controlled terms:

- Spectrum
- Bands
- Fine structure of IR bands
- Intensity of IR bands
- Polarization of IR bands
- Reflection spectrum
- Far IR spectrum
- Near IR spectrum
- Far IR bands
- Near IR bands
- Intensity of far IR bands
- Intensity of near IR bands
- Intensity of rotational lines of IR bands
- Linewidth of IR bands
- Linewidth of rotational lines of IR bands
- IR second moment
- IR-radiofrequency double resonance
- IR-microwave double resonance
- Vibrational relaxation
- Vibrational energy transfer
- Overtone spectrum
- Anisotropy of IR bands
- Fermi resonance
- IR

Interatomic Distance and Angle (GEO)

This field contains information about

- Electron distribution
- Interatomic distances and angles

Ionization Potential (IP)

The ionization potential is defined as the energy per unit charge required to completely removing an electron from an atom or molecule to an infinite distance. The Ionization Potential search field contains the energy values and measurement methods. You can search for the associated information using the parameter field code IP.MET.

Isoelectric Point (IEP)

The isoelectric point is defined as the pH value at which a substance in a solution is electrically neutral.

Isolation from Natural Product (INP)

The Isolation from Natural Product field contains names of the source in nature (plant, fungus, animal etc.) or an industrial grade natural product from which compounds have been isolated. Sources are only recorded when a compound has been isolated. The identification of well-known compounds by instrumental methods (e.g. GLC, TLC) as components of natural or synthetic products is not recorded here (e.g. the identification of pentan-2-one in tobacco smoke or limonene in the ethereal oils of a rare plant or saccharose as a component of a tree-bark extract). Terms do not belong to a controlled vocabulary, specific names (e.g. the systematic name of the plant or animal) are used when they are available.

Kinematic Viscosity (KV)

Kinematic viscosity is a coefficient defined as the ratio of the dynamic viscosity of a fluid to its density. The values are given at specified temperatures. These temperatures can be searched using the associated parameter field code KV.T.

Linearized Structure Formula (LSF)

ReaxysFile contains two Molecular Formula Fields

- Molecular Formula (see MF)
- Linear Structure Formula (/LSF)

LSF is always present for ionic structures and isotopically labeled compounds. It may contain

- Charges
- Isotopes
- The formula of an inorganic compound in linearized format
- The formula of an inorganic fragment in multi-fragment compounds in linearized format.

Examples:

- C4H12N<1+>+Cl<1->
- C3H8(18)O
- C6H7N*H2SO4

Liquid Phase (LIQPH)

This field contains contains information about:

- Rate of evaporation
- Supercoolability
- Structure of the liquid
- Radial distribution function
- Association in the liquid state
- Self-association in solution
- Relaxation time for reorientation
- Rotational correlation time
- Liquid-crystalline properties
- Rotational correlation function of the liquid
- Correlation function of the liquid
- Order parameter
- Liquid-crystalline transition temperatures

Liquid/Liquid System MCS (LLSM)

The field Liquid/Liquid Systems Description (/LLSM.KW) contains keywords from the following list of controlled terms:

- Liquid/liquid phase diagram
- Solution equilibrium
- Critical solution temperature
- Temperature of separation
- Equilibrium of liquid phases
- Distribution between solvent 1 + 2
- Solubility diagram
- Critical mixing temperature(s)
- Critical demixing temperature(s)

Liquid/Solid System MCS (LSSM)

The field Liquid/Solid Systems Description (/LSSM.KW) contains keywords from the following list of controlled terms:

- Liquid/solid phase diagram
- Melting diagram
- Solidification diagram
- Solidification points of mixtures
- Eutectic
- Liquid-solid phase equilibrium
- Melting points
- Glass transition temperature(s)
- Phase transition temperature(s)

Liquid/Vapor System MCS (LVSM)

The field Liquid/Vapor Systems Description (/LVSM.KW) contains keywords from the following list of controlled terms:

- Liquid/vapor phase diagram
- Liquid/vapor equilibrium
- Boiling point diagram
- Boiling points of mixtures
- Vapor pressure diagram for the mixture
- Partial pressures of the components
- Critical data for mixtures
- Activity coefficients of the components in the mixture
- Vapor pressure
- Tricritical point
- Critical temperature
- Critical pressure
- Critical density
- Critical volume
- Fugacities

Luminescence (LUM)

The field Luminescence Description (LUM.KW) contains keywords from a list of controlled terms:

- Emission spectrum in the infrared region
- Radioluminescence
- Sonoluminescence
- Triboluminescence
- Thermoluminescence
- Electroluminescence
- Lasing properties
- Luminescence lifetime
- Luminescence quenching
- Degree of depolarization of luminescence
- Luminescence quantum yield
- Luminescence
- UV/VIS emission spectrum
- UV/VIS emission
- X-ray emission spectrum
- X-ray emission cross-section
- X-ray emission quantum yield
- Luminescence spectrum

Magnetic Data (MAG)

This field contains information about:

- Anisotropy of magnetic susceptibility
- Magnetic moment
- Magnetic properties
- paramagnetic
- Volume susceptibility
- Rotational magnetic moment

Magnetic Susceptibility (MSUS)

Magnetic susceptibility is the ratio of magnetization to field strength.

Markush Reference Count (MARKREF)

Number of referenced Markush structures.

Mass Spectrum (MS)

This field contains keywords from the following list of controlled terms:

- spectrum
- chemical ionization (CI)
- collisional activation
- electron impact (EI)
- electrohydrodynamic ionization
- fast atom bombardment (FAB)
- field desorption
- field ionization
- fragmentation pattern
- high frequency spark
- hydrogen and carbon scrambling
- ion kinetic energy (spectrum) (IKE(S))
- ion current profiles
- laser desorption
- metastable ions
- mass ion kinetic energy (MIKE)
- negative ion spectroscopy
- negative secondary ions
- positive secondary ions
- charge exchange with rare gas ions
- collision-induced dissociation
- doubly charged ions
- ion-cyclotron resonance
- ion impact
- negative chemical ionization
- neutral impact
- Penning ionization
- photoelectron-photoion coincidence
- photoionization
- secondary ions
- charge exchange with negative ions
- neutral fragments
- surface ionization
- single ion monitoring (SIMS)
- liquid secondary ion mass spectrometry (LSIMS)
- neutralization-reionization mass spectrometry (NRMS)
- desorption chemical ionization (DCI)
- time-of-flight mass spectra (TOFMS)
- multiphoton ionization (MPI)
- resonance enhanced multiphoton ionization (REMPI)
- direct electron ionization (DEI)
- tandem mass spectrometry
- collisionally activated dissociation (CAD)
- appearance potentials
- charge exchange with positive ions

Mechanical & Physical Property MCS (MECM)

The field Mechanical & Physical Properties Description (/MECM.KW) contains keywords from the following list of controlled terms:

- Volume change on mixing
- Partial molal volume
- PVT Relationship
- Virial coefficients
- Adiabatic compressibility
- Isothermal compressibility
- Excess partial molal volume
- Apparent molal volume
- Apparent specific volume
- Second virial coefficient(s) of the equation of state
- Third virial coefficient(s) of the equation of state
- Fourth virial coefficient(s) of the equation of state
- Ultrasonic velocity
- Hypersonic velocity
- Ultrasonic absorption
- Hypersonic absorpion
- Acoustic relaxation time

Mechanical Property (MEC)

This field contains information about

- Specific volume
- Volume change on melting
- PVT relationship
- Virial coefficients of the equation of state
- Internal pressure
- Elasticity constants
- Compressibility
- Viscosity
- Molar volume
- Second virial coefficient of the equation of state
- Third virial coefficient of the equation of state
- Fourth virial coefficient of the equation of state

Melting Point (MP)

The melting or freezing point of a pure substance is the temperature at which its crystals are in equilibrium with the liquid phase at atmospheric temperature. You can search for the associated information about e.g. the solvent from which the material whose melting point is mentioned was crystallized using the parameter field code MP.SOL.

Molecular Deformation (DFM)

This field contains information about

- Fundamental vibrations
- Force constants
- Rotational constants
- Centrifugal distortion constant(s)
- Coriolis coupling constant(s)

Molecular Formula (MF)

The Molecular Formula Field contains the complete formula of a substance.

Mutarotation (MUT)

Mutarotation is a change in optical rotation that takes place with time in solutions prepared freshly from optically active substances as a result of the reversible conversion of one isomeric form to another. The values are given at a specified wavelength. You can search for the associated information about the type, concentration, length of path, solvent, wavelength, temperature and time using the parameter field codes.

Nuclear Magnetic Resonance (NMR)

The NMR Spectrum parameter fields are present when the publication contained individual chemical shift values from the NMR spectra for the substances. Some fields are very useful in combination with other queries to refine search strategies. You can search for this associated information using the parameter field codes. The field NMR Description (NMR.KW) contains keywords from the following list of controlled terms:

- Spectrum
- Chemical shifts
- Dynamic NMR
- INDOR
- NMR with shift reagents
- Linewidth of NMR absorption
- NMR in liquid-crystal phase
- NOE
- Second moment of NMR absorption
- Spin-lattice relaxation time (T1)
- Spin-spin relaxation time (T2)
- 2D-NMR
- 3D-NMR
- Aromatic solvent induced shifts
- Radical contact shifts

- Double resonance
- Spin-rotation constant
- 1H-electron double resonance
- CIDNP
- NMR
- Spin-spin coupling constants

Nuclear Quadrupole Resonance (NQR)

The field NQR Description (NQR.KW) contains keywords from a list of controlled terms:

- Nuclear quadrupole resonance
- Nuclear quadrupole coupling constants
- Pure NQR

Number of Fragments (NF)

Number of fragment forming the substance.

Optical Data MCS (ODM)

This field contains information Kerr constant and other optical data.

Optical Rotatory Dispersion (ORD)

Optical rotatory dispersion is defined as the variation in optical rotation with the wavelength of light. The wavelength range over which this phenomenon has been measured is stored in the ORD field

Optical Rotatory Power (ORP)

The optical rotatory power is the ability of a dissymmetric substance to refract and absorb right and left-polarized light to different extents. This results in continuous rotation of the plane of polarization. You can search for the associated information about the type, concentration, and length of path, solvent, wavelength and temperature using the parameter field codes ORP.TYP, ORP.C, ORP.LEN, ORP.SOL, ORP.W and ORP.T.

Optics (OPT)

This field contains information about:

- Crystal refractive indices
- Natural birefringence
- Mechanical birefringence
- Magnetic birefringence (Cotton-Mouton effect)
- Electric birefringence (Kerr effect)
- Diffraction
- Reflection
- Rayleigh scattering
- Degree of depolarization of Rayleigh scattering
- Iso- & anisotropic components of Rayleigh scattering
- Plain curve
- Cotton Effect (abnormal curve)
- Magnetorotation
- Magnetic circular dichroism
- Thermochromism
- Photochromism
- Linear dichroism
- Mutarotation coefficient
- Optical properties
- Rayleigh-Brillouin scattering
- Verdet constant
- Flow birefringence

Other Spectroscopic Methods (OSM)

This field contains information about

- Photoelectron spectrum
- ESCA
- Moessbauer effect
- Electronic state studies
- Electron impact spectrum
- Auger electron spectrum
- Multiple resonance studies

Other Thermochemical Data (OTHE)

This field contains information about:

- Cryoscopic constant
- Ebullioscopic constant
- Enthalpy
- Heat of combustion at constant volume
- Enthalpy of self-association
- Thermodynamic properties
- Heat capacity
- Entropy
- Heat capacity ratio Cp/Cv
- Gibbs free energy

Oxygen Demand (EOD)

Oxygen demand studies are performed to determine the degree of pollution in an effluent of a sewage plant or a body of inland water. Oxygen Demand is differentiated into biochemical oxygen demand and chemical oxygen demand.

Biochemical Oxygen Demand is a measure of the oxygen requirement in microbial oxidation of organic substances contained in water. Usually BOD5 (5 days continuous measurement at 20°C in the dark) is reported.

Chemical Oxygen Demand is a measure of the amount of oxygen required to oxidize organic and oxidizable inorganic compounds in water and wastewater. The amount of oxygen is provided by the addition of potassium dichromate.

Partition octan-1-ol/water MCS (POW)

The partition coefficient constant Pow describes the equilibrium distribution of a substance between n-octanol and water phases. The distribution coefficient is the quotient of two concentrations and is usually given in the form of the decadic logarithm (log POW). You can search for both values POW and log POW. Information on the related temperature is given in the parameter field POW.T.

Patent Information (PI)

Information related to patents, e. g. first claim, secondary claim, application number, filing date, inventor, date of publication, priority number

Patent Specific Data (PSD)

contain information on prophetic substances, related Markush structures and location in patent.

Pharmacological Data (PHARM)

Pharmacological Data

Considering pharma research you are interested to synthesize products (pharmaceuticals) with a defined effect in order to have a therapeutic target.

Pharmacological (and toxicological) Data in ReaxysFile focus on human and mammalian pharmacology and toxicology, i.e. both therapeutic and toxic effects of chemical substances as well as studies on pharmacodynamics and pharmacokinetics are included. Examinations with bacteria or enzymes concerning human pathology are also regarded. All indexed data are stored in a very detailed any.

Toxicological Data

Toxicology studies unwanted effects of chemical and physical agents, including drugs and pollutants on living organisms. The potential for toxicity is accessed during the development of e.g. all new drugs.

Phosphorescence (PHO)

The field Fluorescence Description (FLU.KW) contains keywords from a list of controlled terms:

- Spectrum
- Maxima
- Fluorescence emission cross-section
- Fluorescence quantum yield
- Fluorescence lifetime
- Fluorescence decay kinetics
- Fluorescence self-quenching
- Fluorescence concentration quenching
- Fluorescence quenching
- Degree of polarization of fluorescence
- Excimer fluorescence
- Delayed fluorescence
- Intersystem crossing [singlet->triplet]
- Energy transfer from singlet state
- Fluorescence excitation spectrum
- Fluorescence intensity
- Fluorescence

Purification (PUR)

The Purification field contains words and phrases that describe the method of purification of a substance.

Comments on the purification of a compound are only accepted when the work, or a large section of it, contains unusual purification methods for the compound in question. Natural occurrence and isolation from natural products are entered under /INP (Isolation from Natural Products). The resolution of racemates does not count as an independent preparation. This is entered under the Description of the preparation of the antipodes (via the racemate) as a method of purification.

Quantum Mechanical Calculations (QCC)

The quantum chemical calculations search field refers to quantum chemical calculations performed for a substance. The calculated properties are available in this field together with a classification of the corresponding quantum chemical method of calculation QCC.MET.

Raman Spectrum (RAS)

The field Raman Description (RAS.KW) contains keywords from a list of controlled terms:

- Spectrum
- Bands
- Degree of depolarization of Raman bands
- Hyper-Raman spectrum
- Linewidth of Raman bands
- Low frequency Raman bands
- Low frequency Raman spectrum
- Preresonance Raman spectrum
- Raman intensities
- Raman resonance effect
- Raman second moment
- Rotational fine structure of Raman bands
- Raman

Reaction Data (RX)

Reaction data are clearly separated in two parts, Reaction Identification Data and Reaction Details. All reactions possessing identical Reaction Identification Data, which means reactions with exactly the same reactants and products are combined under one Reaction ID. The total number of reaction variations is given in the field “Number of Reaction Details” (RX.NVAR). Particular facts of a distinct way to carry out a reaction are given in the Reaction Details.

Which methods of preparation are indexed?
Chemical or biochemical methods are only recorded when they are suitable for large-scale preparations. Preparative methods that are complicated or have low yields are acceptable only if they are new and have preparative usefulness. A preparative method is also recorded if there is only one general method given which is applicable to the preparation of several compounds. If a preparative method has a back reference it need not be recorded if it is clear that the same compound has been prepared before by the same method. If it is suspected that the back reference relates only to an analogous preparation of another compound or a general method then the preparation is indexed. The field Reaction Classification (RX.CL) will contain the entry "Preparation".

Which other reactions (chemical behavior) are indexed?
For a reaction to be included and hence classified as "Chemical Behavior" one of the following criteria must be met.

1. There are quantitative results pertaining to the course of a reaction; at least one of the attributes presented should be listed in the field "Subject Studied" (RX.SUB).
2. The investigation of the chemical behavior of the compound is given as the object of the investigation or forms a major part of the publication (this can usually be determined from the abstract of the paper). If the investigation of a new type of reaction forms the basis of the publication and a number of compounds were investigated and the results tabulated only the prototypes are recorded and not higher homologues or substituted compounds. This restriction applies only to qualitative results; quantitative results (e.g. kinetics) are recorded for all the compounds investigated.

Reaction Identification Data
Reaction Identification Data include Reaction ID, which is the unique registry number of the reaction, Reactant Name, Reactant ReaxysFile Record Number (Reactant AN), Product Name and Product ReaxysFile Record Number (Product AN) and give information on reactants and products which are usually registered organic compounds.
In the reaction documents the AN, which identifies an indexed title compound, appears in the Reactant AN (RX.RAN) field for a reactant, while the one of a product is listed in the Product AN (RX.PAN) field.

Reaction Details
Reaction Details provide explicit information about reaction conditions. If quoted in the literature, further information such as yield, reagent, catalyst, solvent, time, temperature, pressure, pH value or reaction type are indexed. Important information which cannot be attributed to other parameter fields, e.g. heating, UV-irradiation or description of biological methods are stored in the “Other Conditions” field.
Depending on the aim of investigation each Reaction Detail is classified either as “Preparation” or as “Chemical Behavior” in the Reaction Classification field (RX.CL). A reaction is ranked as “Preparation” if the investigation focused on the preparative method. “Chemical Behavior” is assigned to data concentrating on thermodynamic or kinetic studies of a reaction. “Multistage” reactions are a special type of preparations where the structures of intermediates are unknown. In this case starting materials for all steps are entered together in the corresponding fields and details for each reaction step are given individually in the single stages.

Refractive Index (RI)

The refractive index is the ratio of the velocity of light in a vacuum to its velocity in the substance. The ratio of the sine of the angle of incidence to the sine of the angle of refraction is the index of refraction of the second medium. The refractive index varies with the wavelength of the incident light, temperature and pressure. The values are given at specified temperature and wavelength.

Related Structure (RSTR)

The Related Structure field contains the ReaxysFile Accession Numbers (AN's) assigned to substances when a new investigation of the cited compound yields different results, e.g. regarding stereochemistry. The entry contains information about the earlier literature reference and a note as to whether the constitution or configuration assigned to the title compound is wrong or doubtful.

Rotational Spectrum (ROT)

The field Rotational Spectrum Description (ROT.KW) contains keywords from a list of controlled terms:

- Microwave spectrum
- Rotational spectrum
- Intensity of microwave bands
- Stark effect
- Rotational-Raman spectrum
- Linewidth of microwave bands
- Intensity of rotational bands
- Linewidth of rotational bands

Self Diffusion (SDIF)

Self-diffusion is defined as the mutual diffusion caused by a concentration gradient (autodiffusion). The values are given at specified temperatures. You can search for this associated information using the parameter field code SDIF.T.

Solubility MCS (SLB)

The solubility of one liquid or solid in another is the mass of a substance contained in a solution, which is in equilibrium with an excess of the substance at a specified temperature. You can search for the associated information about the saturation, the temperature, the solvent and the ratio of solvents using the parameter field codes SLB.SAT, SLB.T, SLB.SOL and SLB.RAT.

Solubility Product MCS (SLBP)

The solubility product is the product of the concentrations of the ions of a substance in a saturated solution of the substance at a specified temperature. You can search for the associated information about the temperature, the solvent and the ratio of solvents using the parameter field codes SLBP.T, SLBP.SOL and SLBP.RAT.

Solution Behavior MCS (SOLM)

The field Solution Behavior Description (/SOLM.KW) contains keywords from the following list of controlled terms:

- Dissolving capacity
- Miscibility
- Solubilizing
- Mutual solubility
- Rate of dissolution
- Solubility [Bunsen absorption coefficient]
- Solubility [Henry constant]
- Solubility [Ostwald absorption coefficient]

Stability in Soil (ECS)

The property characterizes the resistance or stability of a substance in the soil. Standardized soils are often used for measurement of specific dissipation times, after which 50, 90 or x% of a substance in a particular soil has disappeared.

Sublimation Point (SP)

The sublimation point is defined as the temperature at which the vapor pressure above a solid is equal to a specified pressure.

Surface Tension (ST)

Surface tension is the force per unit length required to create a new unit area of gas-liquid interface. You can search for information about the associated temperature using the parameter field code ST.T.

Thermal Expansion (TEC)

The thermal expansion coefficient is the ratio of the change in length per unit length or change in volume per unit volume to the change of temperature. The coefficient field is linked to the associated temperature and to the kind of expansion.

Transition Point of Liquid Modification (LPTP)

The temperature at which compounds undergo phase transition in the liquid phase is called the liquid phase transition point. The LPTP field contains the temperature values for the substances. The names of the phases (i.e. nematic, isotropic, crystalline, cholesteric, etc.) are given in the note field.

Transport Data (TRAN)

This field contains information about:

- Thermal conductivity
- Rotational diffusion constant(s)
- Thermal diffusion

Transport Phenomena MCS (TRAM)

The field Transport Phenomena Description (/TRAM.KW) contains keywords from the following list of controlled terms:

- Viscosity
- Diffusion
- Thermal diffusion
- Dynamic viscosity
- Kinematic viscosity
- Bulk viscosity
- Diffusion coefficient
- Binary diffusion coefficient
- Interdiffusion
- Thermal diffusion factor
- Thermal diffusion (Soret coefficient)
- Diffusion thermo effect (Dufour effect)
- Thermal conductivity

Triple Point (TP)

The triple point is the point in a phase diagram where three phases of a substance exist at equilibrium and is fully defined by the temperature and pressure at that point. The Triple Point field contains the temperature values for the substances.

Type of Substance (CTYPE)

The following substance types are available and can be used for filtering:

- Acyclic
- Alloy
- Biomolecule
- Coordination compound
- Glass or ceramic material
- Heterocyclic
- Isocyclic
- Isotope or isotope containing compound
- Markush structure
- Mineral
- Composition completely given)
- Mixture (composition not given)
- Mixture (composition partially given)
- Polymer (monomers given)
- Polymer (monomers not given)
- Solid solution

Use of Compound (USC)

and Handling describes the use of a substance in the preparative chemistry, in the laboratory and contains information on safety aspects or the attainment of the desired effect, such as phase transfer catalysis, reduction, quenching, etc.

UV and Visible Spectrum (UVS)

The field UV Description (UVS.KW) contains keywords from a list of controlled terms:

- Spectrum
- Absorption maxima
- Reflection spectrum
- Singlet-triplet band
- Solvatochromism
- Triplet-triplet band
- Vacuum-UV spectrum
- Absorption spectrum
- Absorption cross-section
- UV excited state absorption
- UV two-photon absorption
- Triplet-singlet absorption spectrum
- Opto-acoustic UV spectrum
- UV/VIS reflection maximum(a)
- X-ray absorption spectrum
- X-ray absorption cross-section
- Band anisotropy
- Oscillator strength
- UV/VIS

Vapor Pressure (VP)

The vapor pressure of a pure liquid or solid is the pressure of the vapor that is in equilibrium with it at a given temperature. You can search for the associated temperature using the parameter field code VP.T.

STN Service Centers

In Europe

FIZ Karlsruhe
STN Europe
P.O. Box 2465
76012 Karlsruhe
Germany

Phone: +49 7247 808-555
Fax: +49 7247 808-259
helpdesk@fiz-karlsruhe.de
www.stn-international.de

In North America

CAS
STN North America
P.O. Box 3012
Columbus, Ohio 43210-0012 U.S.A.

CAS Customer Care:
Phone: 800 753 4227 (North America)
614 447 3700 (worldwide)
Fax: 614 447 3751
help@cas.org
www.cas.org

In Japan

JAICI (Japan Association for
International Chemical Information)
STN Japan
Nakai Building
6-25-4 Honkomagome, Bunkyo-ku
Tokyo 113-0021, Japan

Phone: +81 3 5978-3601 (Technical Service)
+81 3 5978-3621 (Customer Service)
Fax: +81-3-5978-3600
support@jaici.or.jp (Technical Service)
customer@jaici.or.jp (Customer Service)
www.jaici.or.jp

FIZ Karlsruhe
Leibniz Institute for Information Infrastructure