

DETERM

Subject Coverage	<ul style="list-style-type: none"> • Bibliographic Information • Data Type Information • Electric Properties • Electrochemical Properties • Identification of Substance • Multi-Component System Properties • Property Relation Information • State-of-System Information • Surface Properties • Thermodynamic Properties • Transport Properties 																									
File Type	Factual, numeric																									
Features	<table border="0" style="width: 100%;"> <tr> <td>Thesaurus</td> <td>Chemical Name (/CN)</td> <td></td> <td></td> <td></td> </tr> <tr> <td>Alerts (SDIs)</td> <td>Not available</td> <td></td> <td></td> <td></td> </tr> <tr> <td>CAS Registry Numbers®</td> <td><input checked="" type="checkbox"/></td> <td>Page Images</td> <td><input type="checkbox"/></td> <td>STN AnaVist <input type="checkbox"/></td> </tr> <tr> <td>Keep & Share</td> <td><input type="checkbox"/></td> <td>SLART</td> <td><input type="checkbox"/></td> <td>STN Easy <input type="checkbox"/></td> </tr> <tr> <td>Learning Database</td> <td><input type="checkbox"/></td> <td>Structures</td> <td><input type="checkbox"/></td> <td>STN Viewer <input type="checkbox"/></td> </tr> </table>	Thesaurus	Chemical Name (/CN)				Alerts (SDIs)	Not available				CAS Registry Numbers®	<input checked="" type="checkbox"/>	Page Images	<input type="checkbox"/>	STN AnaVist <input type="checkbox"/>	Keep & Share	<input type="checkbox"/>	SLART	<input type="checkbox"/>	STN Easy <input type="checkbox"/>	Learning Database	<input type="checkbox"/>	Structures	<input type="checkbox"/>	STN Viewer <input type="checkbox"/>
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Record Content	<ul style="list-style-type: none"> • Thermophysical data • Bibliographic information, indexing terms, property codes, substance information abstracts, chemical names and CAS Registry Numbers® 																									
File Size	843,076 records (03/2011)																									
Coverage	1819-present																									
Updates	Irregular																									
Language	English																									
Database Producer	DECHEMA e.V. Theodor-Heuss-Allee 25 60486 Frankfurt am Main Germany Phone: +49 69 7564-0 Fax: +49 69 7564-201 Copyright Holder																									

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 - Dissertations
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 - Standards
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- User Aids**
- Online Helps (HELP DIRECTORY lists all help messages available)
 - STNGUIDE
-

- Clusters**
- ALLBIB
 - AUTHORS
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 - CASRNS
 - NUMERIC
- [STN Database Clusters](#) information (PDF).
-

Pricing See the [STN Price List](#) or enter HELP COST at an arrow prompt.

Search and Display Field Codes

There are bibliographic records and factual table records in DETERM. After a search in bibliographic fields only the bibliographic fields can be displayed. To see corresponding tables (including Substance Identification and Data Information fields) use the SELECT TABLE command. A search with the E-number will retrieve all tables related to this bibliography. After a search in factual fields the corresponding bibliographic record can be displayed with the predefined formats BIB or ALL. For the display of single bibliographic fields search for the corresponding bibliographic record first. Use the SELECT BIBLIO command followed by a search of the resulting E-number.

There are no fields that allow left truncation in this file.

General Search Fields

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index (contains single words from title (TI), abstract (AB), as well as CAS Registry Numbers (RN))	None or /BI	S STEREO? S 5673-09-6 S BIVALENT TRANSITION METAL#	TI, AB, RN
Accession Number	/AN	S 1-1005/AN	AN
Author	/AU	S GMEHLING, J/AU	AU
Classification Code	/CC	S LLE/CC	CC
Document Type	/DT	S DISSERTATION/DT	DT
File Segment (1)	/FS (or /TC)	S ELДАР/FS	FS
International Standard Document Number (CODEN)	/ISN	S ACAPCT/ISN	SO
Journal Title	/JT	S AICHE J/JT	JT
Language (ISO code and text)	/LA	S SPANISH/LA S ES/LA	LA
Publication Year (2)	/PY	S 1985<PY<1991	PB
Source (contains CODEN, volume, issue, page and single words from journal title) (1)	/SO	S AJCHAS/SO S J CHEM SOC FARADAY/SO	SO
Title	/TI	S SURFACTANT/TI S MASS ACTION MODEL/TI	TI
Update Date (2)	/UP (or /ED)	S L3 AND UP>=2007	UP

(1) A search can be restricted to one file segment. For online 'HELP' on this subject type 'HELP RANGE' at an arrow prompt (=>).

(2) Numeric search field that may be searched with numeric operators or ranges.

Substance Identification

Search Field Name	Search Code	Search Examples	Display Codes
Accession Number	/AN	S 2-1004/AN	AN
Atom Count (1)	/ATC	S 2/ATC	from MF
Chemical Name (2)	/CN	S FERROCENE/CN	CN
Chemical Name Segment (3)	/CNS	S IRON/CNS	from CN
Element Count (total) (1)	/ELC	S 1/ELC	from MF
Element Count (1)	/Elem. Symbol	S 4/CL	from MF
Element Symbol	/ELS	S CU/ELS	from MF
Field Availability	/FA	S COLUMN?/FA	FA
Molecular Formula	/MF	S CHCL3/MF	MF
Number of Components (Substances) (1)	/NC	S 1/NC	IDE

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Substance Identification (cont'd)

Search Field Name	Search Code	Search Examples	Display Codes
Periodic Group CAS Registry Number Substance Descriptor System Description (4)	/PG /RN /SDC /SYST	S LNTH/PG S 271-89-6/RN S "RUHRGEBIET/REGION"/SDC S I40/SYST	from MF RN IDE IDE

- (1) Numeric search field that may be searched with numeric operators or ranges.
 (2) CA index names and synonyms are indexed. For pseudocomponents the pseudocomponent name is indexed. For coal and coal liquids the systematic name is indexed. A thesaurus is available for /CN featuring molecular formulas, CAS Registry Numbers and synonym names.
 (3) The /CNS field does not contain parsed segments of the synonyms.
 (4) Codes or bound phrases are used as search terms. The following codes are available:

1st digit of the code **Bound Phrase**

O	organic
I	inorganic
M	organometallic
X	mixed organic-inorganic
A	organic-organometallic
B	inorganic-organometallic
C	inorganic-organic-organometallic
E	EMF cell

2nd digit of the code **Bound Phrase**

1	pure compound
2	binary system
3	ternary system
4	quaternary system
5	quinary system
6	senary system
7	septenary system
8	octanary system
9	novenary system
0	denary system

3rd digit of the code **Bound Phrase**

O	no reaction
A	association
C	chemical reaction
D	dissociation
T	phase transition
E	electrolyte

Data Information

Search Field Name	Search Code	Search Examples	Display Codes
Data Type (1) Property (2,4) (Preferred Property Name)	/DATA /PROP (or /PPN)	S MOLAR PROPERTY/DATA S HCP/PROP S HEAT CAPACITY/PROP S VISCOSITY/PPN	COL COL, TBL, TBLO
Property Relation (1)	/PROPRL	S L2(S)PARTIAL EXCESS PROPERTY COMPOUND 1/PROPRL	COL
Row Counter (Table Lines) (3)	/ROW	S L7 AND ROW>10	ROW
Description of State (class, type, relation, condition) (1)	/STATE	S EUTECTIC/STATE	COL

- (1) Use the EXPAND command to see valid search terms.
 (2) Use the EXPAND command to see a list of the properties available. Valid search terms are property names and codes.
 (3) Numeric search field that may be searched with numeric operators or ranges.
 (4) The following properties are numerically searchable:

STN Code	Property	Default Unit	Further Unit
DEN	Density	kg/m**3	
HCP	Heat Capacity	J/mol*K	J/kg*K
PRES	Pressure	Pa	
TCND	Thermal Conductivity	W/m*K	
TEMP	Temperature	K	
VS	Viscosity	Pa*s	m**2/s
XL	Liquid Concentration	mol/m**3	volfrac, wgtfrac, mol/kg, molfrac

For numeric searches of properties only the STN code is allowed as search code. Search can be done with or without unit. If no unit is assigned, the search is done using the defaults. If an invalid unit is chosen you will get an error message including the right unit(s).

Chemical Name (/CN) Thesaurus

Code	Content	Examples
ALL	All Associated Terms (MF, SELF, RN, USE, UF)	E BORON TRIHYDROXIDE+ALL/CN
PFT	All Preferred and Forbidden Terms	E CESIUM BROMATE+PFT/CN
UF	Used For Terms (Forbidden Terms)	E BROMIC ACID CESIUM SALT+UF/CN
USE (1)	Use Terms (Preferred Terms)	E MAGNESIUM BROMIDE+USE/CN

(1) Automatic Relationship is SET OFF. In case of SET REL ON the result of EXPAND or SEARCH without any relationship code is the same as described for AUTO.

Thesaurus Field Descriptors

Code	Description
--->	Self
MF	Molecular Formula
RN	CAS Registry Number
UF	Used For (forbidden term)
USE	Use Term (preferred term)

DISPLAY and PRINT Formats

Search results may be displayed by specifying the individual display field, list of fields, predefined display formats, list of formats or a combination of these. Multiple codes must be separated by commas or spaces. The fields are displayed or printed in the order requested.

There are bibliographic records and table records in DETERM. After a search in Substance Identification or Data Information fields the corresponding bibliographic record can be displayed with the predefined format BIB. For the display of single bibliographic fields you have to search for the corresponding bibliographic record first. Use the SELECT BIBLIO command followed by a search of the resulting E-number. After a search in bibliographic fields only the bibliographic fields can be displayed. To see corresponding tables (including Substance Identification and Data Information fields) use the SELECT TABLE command. A search with the E-number will retrieve all tables related to this bibliography.

The default format in the DETERM database is the dynamic display format QRD (Query Related Data) providing display fields in which your search term appears (HIT) and related information. Hit term highlighting is available for all display formats. Highlighting must be ON during SEARCH to use the HIT and QRD formats.

DISPLAY and PRINT Formats (cont'd)

Format	Content	Examples
AB AN AU CC DT FS ISN JT LA PY RACC SO TI UP (1)	Bibliographic fields: Abstract Accession Number Author Classification Code Document Type File Segment International Standard (Document) Number (CODEN) Journal Title Language Publication Year Related Accession Number Source Title Update Date	D AB D AN D AU D CC D DT D FS D ISN D JT D LA D PY D RACC D SO D TI D UP
CN MF RN SYST	Identification of Substance fields: Chemical Name Molecular Formula CAS Registry Number System Description	D CN D MF D RN D SYST
ROW	Data Information: Row Counter (Table Lines)	D ROW
ALL ALLO BIB COL IDE QRD (2) TBL TBLO TRIAL	All Data (BIB, IDE, COL, TBL) All Data (BIB, IDE, COL, TBLO) Bibliography (AB, AN, AU, CC, DT, FS, LA, PY, RACC, SO, TI) Column Description (PROP, PROPRL, DATA, STATE) Identification of Substance Query Related Data (default: dynamic format HIT and relating information) Column Description and Data Table (SI Units) Column Description and Data Table (Original Units) AN, CN, PROP, ROW; system parameters like temperature, pressure, concentration; number of table hit lines	D ALL D ALLO D BIB D COL D IDE D QRD D TBL D TBLO D TRIAL
HIT	Hit term(s) and field(s)	D HIT

(1) Custom display only.

(2) The relation of display fields in QRD to the searched fields is given below:

Search Field(s)	Display fields in QRD
AN	AN
AU, BI*, CC, DT, LA, PY, TI	AN, BIB**
FS	AN, FS, RACC
ISN, JT or SO	AN, BIB**, SO
ROW	FA
ATC, CN, CNS, ELC, Element Symbol, ELS, MF, NC, PG, RN, SDC or SYST	AN, IDE
PROP, PROPR, DATA, STATE	AN, COL
Numeric Search	AN, IDE, TBL

* Terms from AB.

** Note: For QRD the meaning of BIB is somewhat different from the predefined format BIB. In the case of QRD the meaning is: AB, AU, CC, DT, FS, LA, PY, RACC, TI.

SELECT, ANALYZE, and SORT Fields

The SELECT command is used to create E-numbers containing terms taken from the specified field in an answer set.

The ANALYZE command is used to create an L-number containing terms taken from the specified field in an answer set.

The SORT command is used to rearrange the search results in either alphabetic or numeric order of the specified field(s).

Additionally, when using a table format with DISPLAY or PRINT, you may sort the answers by the data columns. The sortable table formats in DETERM are within TBL and TBLO. The following syntax has to be used:

For TBL:

=> D TBL TSORT=(DATSI,Cx, sort order)

For TBLO:

=> D TBLO TSORT=(DATOR,Cx, sort order)

where x is the number of the column to be sorted and the sort order is given as 'A' for ascending and 'D' for descending. If no sort order is given the default ('A') is used.

Field Name	Field Code	ANALYZE/ SELECT (1)	SORT
Abstract	AB	Y (2)	N
Author	AU	Y	Y
CAS Registry Number	RN	Y	N
Chemical Name	CN	Y	Y
Classification Code	CC	Y	Y
Data Type	DATA	Y	N
Description of State	STATE	Y	N
Document Type	DT	Y	Y
File Segment	FS	Y	N
International Standard (Document) Number (CODEN)	ISN	Y	N
Journal Title	JT	Y	N
Language	LA	Y	Y
Molecular Formula	MF	Y	N
Property	PROP	Y	N
Property Relation	PROPRL	Y	N
Publication Year	PY	Y	Y
Row Counter (Number of Table Lines)	ROW	Y	N
System Description	SYST	Y	N
Title	TI	Y	Y

(1) HIT may be used to restrict terms extracted to terms that match the search expression used to create the answer set, e.g., SEL HIT AB.

(2) Appends /BI to the terms created by SELECT.

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Sample Records

DISPLAY ALL

Bibliography for Table Number: 20-103982 DDB PURE
 Accession Number (AN): 19-16027 DETHERM
 Related Acc. No. (RACC): Tables: 20-103979 - 20-103982
 Title (TI): Vapor-Liquid Equilibria of Binary Mixtures of
 Hexane or 1-Hexene with Ethyl Acetate or Vinyl
 Acetate
 Author (AU): Beck, C.; Duvigneaud, F. A.; Murphy, C. D.
 Source (SO): Private Communication, 1-26
 Document Type (DT): Miscellaneous
 Language (LA): English
 Classification Code (CC): PRP: All properties (general)

Identification of System

System Description (SYST): 010 organic, pure compound
 Substance (1) of (1):
 Chemical Name (CN): Acetic acid ethenyl ester
 Synonyms: Vinyl acetate; Ethenyl ethanoate;
 Ethenyl acetate; Ethanoic acid ethenyl ester;
 Acetic acid vinyl ester
 Molecular Formula (MF): C4 H6 O2
 CAS Reg. Number (RN): 108-05-4

Data Information

Property (1) of (2):
 Property (PROP): BP boiling point (boiling temperature,
 bubble temperature, temperature)
 Original Unit: K
 SI Unit : K
 Data Type (DATA): experimental value
 Desc. of State (STATE): vapor-liquid equilibrium; saturated condition

Property (2) of (2):
 Property (PROP): VP vapor pressure
 Original Unit: kPa
 SI Unit : Pa
 Data Type (DATA): experimental value
 Desc. of State (STATE): vapor-liquid equilibrium; saturated condition

SI UNIT VALUES

1:	2:
BP	VP
(K)	(Pa)
313.15	29130.9
313.15	29242.9
323.15	43711.1
323.15	43741.7

Billing Class: 1

EXPAND IN CHEMICAL NAME THESAURUS

=> E FLUORANTHENE+ALL/CN

```
E1          MF    C16 H10/CN
E2          130    --> Fluoranthene/CN
E3          RN    206-44-0/CN
            UF    1,2-Benzacenaphthene
            UF    Idryl
***** END *****
```

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