



STN is operated in North America
by Chemical Abstracts Service.

STN Database Summary Sheet

DETERM is a factual database that contains thermophysical data important for the design of various processes in the chemical industry. More than 500 properties are covered for pure compounds, as well as for mixtures of defined composition. Considered are about 20,000 inorganic and organic substances, including the most important technical chemical compounds, the most important compound classes, and the most important homologous classes.

For most of the substances, CAS Registry Numbers are available. The database is in English and consists of two types of document units: factual records (data tables) and citations. Several factual records may be related to one citation.

A thesaurus is present for the Chemical Name (/CN) field featuring molecular formulas, CAS Registry Numbers, and synonym names.

Subject Coverage

- Identification of Substance
- Thermodynamic Properties
- Multicomponent System Properties
- Electric Properties
- Transport Properties
- Surface Properties
- Electrochemical Properties
- Property Relation Information
- Data Type Information
- State-of-System Information
- Bibliographic Information

Sources

- Journals
- Conference contributions
- Handbooks
- Manufacturers' data
- Dissertations
- Reports
- Standards

File Data

- 1819 to the present
- More than 593,700 records for data tables (2/06)
- More than 65,100 records for bibliographic information (2/06)
- Updated twice a year at irregular intervals
- Automatic current-awareness searches (SDIs) are not available

User Aids

- DETERM Database Description
- Online Helps (HELP DIRECTORY lists all help messages available)
- STNGUIDE

Database Producer/Supplier

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DETERM

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.

Bibliographic Fields

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index (contains single words from the title (TI) and abstract (AB) fields, as well as CAS Registry Numbers)	None (or /BI)	S STEREO? S 5673-09-6 S BIVALENT TRANSITION METAL	AB, RN, TI
Accession Number	/AN	S 0-120/AN	AN
Author	/AU	S GMEHLING, J/AU	AU
Classification Code	/CC	S LLE/CC S LIQUID/CC S OPTIC PROPERTIES/CC	CC
Document Type (code and text)	/DT (or /TC)	S DISSERTATION/DT S D/DT	DT
Field Availability	/FA	S L1 AND AB/FA	FA
File Segment (1)	/FS	S ELDAR/FS	FS
International Standard (Document) Number (CODEN)	/ISN	S ACAPCT/ISN	ISN, SO
Journal Title	/JT	S ADVAN CHEM SER/JT	JT, SO
Language (code and text)	/LA	S SPANISH/LA S ES/LA	LA
Publication Year (2)	/PY	S 1985<PY<1991	PY
Source (contains journal title, CODEN, volume, issue, page)	/SO	S AJCHAS/SO S J CHEM SOC FARADAY/SO S (FARADAY AND 82 AND 5)/SO	SO
Title	/TI	S SURFACTANT/TI S MASS ACTION MODEL/TI	TI
Update Date (2)	/UP (or /ED)	S L3 AND UP>=19960600	UP

(1) A search can be restricted to one file segment with SEARCH RANGE or SET RANGE. Enter HELP RANGE at an arrow prompt (=>) in DETERM for details. Enter HELP FS for more information on the file segments in DETERM.

(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 Atom Count (1) CAS Registry Number Chemical Name (2)	/AN /ATC /RN /CN	S 2-1004/AN S 2/ATC S 271-89-6/RN S FERROCENE/CN S ACETYL BROMIDE/CN S C11 H10+ALL/CN	AN MF RN CN
Chemical Name Segment (3) Element Count (1)	/CNS /Element Symbol	S IRON/CNS S 4/CL	CN MF
Element Count (total) (1) Element Symbol Field Availability	/ELC /ELS /FA	S 1/ELC S CU/ELS S COLUMN?/FA S L1 AND RN/FA	MF MF FA
Molecular Formula	/MF	S CHCL3/MF S C H CL3/MF	MF
Number of Components (1) (Substances)	/NC	S 1/NC	SYST
Periodic Group Substance Descriptor	/PG /SDC	S LNTH/PG S "RUHRGEBIET/REGION"/SDC	MF SDC
System Description (4)	/SYST	S I40/SYST	SYST

(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	Bound Phrase	2nd digit	Bound Phrase	3rd digit	Bound Phrase
O	organic	1	pure compound	0	no reaction
I	inorganic	2	binary system	A	association
M	organometallic	3	ternary system	C	chemical reaction
X	mixed organic-inorganic	4	quaternary system	D	dissociation
A	organic-organometallic	5	quinary system	T	phase transition
B	inorganic-organometallic	6	senary system	E	electrolyte
C	inorganic-organic-organometallic	7	septenary system		
		8	octanary system		
E	EMF cell	9	novenary system		
		0	denary system		

DETERM**Data Information**

Search Field Name	Default Unit	Search Code	Search Examples	Display Codes
Data Type (1) Density (2,3)	— kg/m**3	/DATA /DEN	S MOLAR PROPERTY/DATA S 27/DEN S L1 AND DEN/PROP S EUTECTIC/STATE	DATA PROP
Description of State (1) (class, type, relation, condition) Heat Capacity (2,3,4)	— J/mol*K	/STATE /HCP	S 44<HCP<50 S L3 AND HCP/PROP S .2/XL S L7 AND XL/PROP	STATE PROP
Liquid Concentration (2,3,5)	mol/m**3	/XL	S 2.5E+05/PRES S PRES/PROP	PROP
Pressure (2,3)	Pa	/PRES	S HCP/PROP S HEAT CAPACITY/PROP S VISCOSITY/PPN	PROP
Property (6) (Preferred Property Name)	—	/PROP (or /PPN)	S L2(S)PARTIAL EXCESS PROPERTY COMPOUND 1/PROPRL	PROPRL
Property Relation (1)	—	/PROPRL	S L7 AND ROW>10 S L6 AND TEMP>=600 S L5 AND TEMP/PROP	Row PROP
Row Counter (3) (Table Lines) Temperature (2,3)	— K	/ROW /TEMP	S TCND<=.06 S TCND/PROP	PROP
Thermal Conductivity (2,3)	W/m*K	/TCND	S VS>5 M**2/S S TEMP/PROP AND VS/PROP	PROP
Viscosity (2,3,6)	Pa*s	/VS		

(1) Use the EXPAND command to see valid search terms.

(2) Search can be done with or without a unit. If no unit is entered, the search is done using the default. If you use an invalid unit, you will get an error message that indicates the correct unit.

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

(4) J/kg*K is also a valid unit in this field.

(5) volfrac, wtfrac, mol/kg, molfrac are also valid units in this field.

(6) Use the EXPAND command to see a list of the properties available. Valid search terms are property names and codes.

(7) m**2/s is also a valid unit in this field.

Thesaurus Field (/CN)

All Relationship Codes can be used with both the SEARCH and EXPAND command in the Chemical Name (/CN) field.

Relationship Code	Content	Example
ALL AUTO (1) PFT UF USE	All Associated Terms (MF, SELF, RN, USE, UF) Use Terms (Preferred Terms) (SELF, USE) All Preferred and Forbidden Terms (SELF, USE, UF) Used For Terms (Forbidden Terms) (SELF, UF) Use Terms (Preferred Terms) (SELF, USE)	E BORIC ACID (H3BO3)+ALL/CN E CESIUM BROMATE+PFT/CN E BROMIC ACID CESIUM SALT+UF/CN E MAGNESIUM BROMIDE+USE/CN

(1) Automatic Relationship Code is SET ON by default. 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

Any combination of display formats listed below may be used to display or print answers. Multiple codes must be separated by spaces or commas. The fields are displayed 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 using the BIB format. To display individual bibliographic fields, search for the corresponding bibliographic record first. Then SELECT BIBLIO. Search the resulting E-number.

After search in bibliographic fields, only the bibliographic fields can be displayed. To see the corresponding tables (including Substance Identification and Data Information fields), enter SELECT TABLE. Search the resulting E - number to 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 fields except AN and RACC. Highlighting must be ON during SEARCH in order to use the HIT and QRD formats.

Bibliographic Information

Format	Content	Examples
AB (1)	Abstract	D AB
AN (1)	Accession Number	D AN
AU (1)	Author	D AU
CC (1)	Classification Code	D CC
DT (1)	Document Type	D DT
FS (1)	File Segment	D FS
ISN	International Standard (Document) Number (CODEN)	D ISN
JT	Journal Title	D JT
LA (1)	Language	D LA
PY (1)	Publication Year	D PY
RACC (1)	Related Accession Number	D RACC
SO	Source	D SO
TI (1)	Title	D TI
UP (1)	Update Date	D UP

Identification of Substance

Format	Content	Examples
CN	Chemical Name	D CN
MF	Molecular Formula	D MF
RN	CAS Registry Number	D RN
SYST	System Description	D SYST

DETERM**Data Information**

Format	Content	Examples
ROW (1)	Row Counter (Table Lines)	D ROW

Predefined Formats

Format	Content	Examples
ALL	AN, FS, RACC, TI, AU, SO, DT, LA, AB, CC, SYST, CN, MF, RN, Properties, Data, State, SI Unit Values table	D 1,3 ALL
ALLO	ALL, with Original Values table	D 1 3 ALLO
BIB	AN, FS, RACC, TI, AU, SO, DT, LA, AB, CC PY, RACC, SO, TI)	D BIB
COL	Properties, Date, State	D L2 COL
FA	Table of fields that contain data for a record	D FA
IDE	AN, SYST, CN, MF, RN, Substance Description	D 1-3,6 IDE
TBL	COL and SI Units Data Table	D TBL
TBLO	COL and Original Units Data Table	D L2 TBLO
TRIAL (1)	AN, System (CN), Data, Property, Table Lines (ROW)	D 1- TRIAL
HIT	Fields containing hit terms	D HIT
QRD (2)	HIT and related fields (QRD is the default)	D QRD L1

(1) No online display fee for this format.

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

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

* Terms from AB.

SELECT, ANALYZE, and SORT Fields

The SELECT command is used to create E-numbers or an L-number 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 table information in TBL and TBLO.

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 specified as A (Ascending) or D (Descending). If no sort order is specified, A is used.

Field Name	Field Code	ANALYZE/ SELECT(1)	SORT
Abstract	AB	Y (2)	N
Accession Number	AN	Y (3)	N
Author	AU	Y	Y
CAS Registry Number	RN	Y (default)	N
Chemical Name	CN	Y	N
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	ISN	Y (4)	N
Journal Title	JT	Y (5)	N
Language	LA	Y	Y
Molecular Formula	MF	Y	N
Property	PROP	Y	N
Property Relation	PROPRL	Y	N
Publication Year	PY	Y	Y
Related Accession Number	RACC	Y (3)	N
Row Counter	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 TI.

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

(3) SELECT HIT and SELECT ANALYZE are not valid with this field.

(4) Selects or analyzes the CODEN with /ISN appended to the terms created by SELECT.

(5) Appends /SO to the terms created by SELECT.

DETERM**Sample Records****DISPLAY ALL**

Bibliography for Table Number: 12-41207 INFOTHERM
 Accession Number (AN): 11-4479 DETERM
 Related Acc. No. (RACC): Tables: 12-41200 - 12-41218
 Title (TI): EXCESS ENTHALPIES OF (METHYL FORMATE OR
 NITROETHANE + AN N-ALKANE) AND OF
 (NITROMETHANE + BUTAN-1-OL OR HEXAN-1-OL OR
 ETHAN-1,2-DIOL)
 Author (AU): FENG, H.; WANG, Y.; SHI, J.
 Source (SO): J. Chem. Thermodyn., (1991), 23, 2, 169-174
 CODEN: JCTDAF
 Document Type (DT): Article
 Language (LA): English
 Abstract (AB): PURITIES OF ALKANES: 99.5 ML%, OF THE OTHER
 COMPOUNDS: 99 ML%.
 Classification Code (CC): HMX: Enthalpies of mixing

Identification of System

System Description (SYST): O20 organic, binary system
 Substance (1) of (2):
 Chemical Name (CN): Nitroethane
 Molecular Formula (MF): C2 H5 N O2
 CAS Reg. Number (RN): 79-24-3

Substance (2) of (2):
 Chemical Name (CN): Hexane
 Synonyms: n-Hexane
 Molecular Formula (MF): C6 H14
 CAS Reg. Number (RN): 110-54-3

Data Information

Property (1) of (3):
 Property (PROP): TEMP temperature
 Original Unit: K
 SI Unit : K
 Data Type (DATA): general value

Property (2) of (3):
 Property (PROP): XL concentration liquid phase
 (concentration)
 Original Unit: mole fraction
 SI Unit : mole fraction
 Prop. Relation (PROPRL): related to compound 1
 Data Type (DATA): general value
 Desc. of State (STATE): liquid state

Property (3) of (3):
 Property (PROP): HREF enthalpy (heat)
 Original Unit: J/mol
 SI Unit : J/mol
 Prop. Relation (PROPRL): excess property
 Data Type (DATA): experimental value
 Desc. of State (STATE): liquid state; isothermic condition

DISPLAY ALL (cont'd)

SI UNIT VALUES

1: TEMP (K)	2: XL (mole fraction)	3: HREF (J/mol)	ERROR HREF (%)
308.15	0.0715	651.	1.
308.15	0.1075	932.	1.
308.15	0.1842	1291.	1.
308.15	0.2143	1398.	1.
308.15	0.2433	1489.	1.
308.15	0.3554	1654.	1.
308.15	0.4550	1716.	1.
308.15	0.5354	1715.	1.
308.15	0.6134	1676.	1.
308.15	0.6764	1588.	1.
308.15	0.7322	1465.	1.
308.15	0.7939	1267.	1.
308.15	0.8452	1051.	1.
308.15	0.8652	946.	1.
308.15	0.8916	788.	1.
308.15	0.9401	471.	1.

Billing Class: 3

EXPAND in /CN Thesaurus

=> **E ARSENOUS TRICHLORIDE+ALL/CN**

```

E1          MF   As Cl3/CN
E2          55   -> Arsenous trichloride/CN
E3          RN   7784-34-1/CN
              UF   Arsenic chloride (AsCl3)
              UF   Arsenic trichloride
              UF   Arsenic-III-chloride
***** END *****

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