

ReaxysFile

Subject Coverage	<ul style="list-style-type: none"> • Chemical data • Electrochemical behaviour • Electrical and magnetic properties • Identification of substance • Multi-component systems • Optical properties • Pharmacological and ecological data • Physical and mechanical properties • Reactions • Safety data • Spectroscopic data • State of aggregation • Structure and energy parameters • Thermodynamic properties • Transport phenomena 		
File Type	Structure, Numeric		
Features	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 checked="" type="checkbox"/> STN Viewer <input type="checkbox"/>
Record Content	<ul style="list-style-type: none"> • The organic substance records contain the critically reviewed and evaluated documents from Handbook of Organic Chemistry as published by Friedrich Beilstein as well as well as data from 176 leading journals in organic chemistry covering the period from 1771 to the present. • A substance record contains structure diagram, the CAS Registry Number, molecular formula etc., all of which are searchable and displayable. • Also searchable and displayable in the ReaxysFile is information on physical and chemical data as well as pharmacological and ecological data for a specific substance. • Some text fields also contain German terms. 		
File Size	10,654,725 substance records (12/10)		
Coverage	1771-present		
Updates	Quarterly		
Language	English, German		
Database Producer	Elsevier Information Systems GmbH Theodor-Heuss-Allee 108 60486 Frankfurt am Main Germany Phone: +49 69 5050 4252 Fax: +49 69 5050 4254	Copyright Holder:	Elsevier Properties SA Espace de l'Europe 3 CH-2000, Neuchâtel Switzerland

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Sources

- 176 Chemistry Journals
 - Handbook of Organic Chemistry (published by F. Beilstein)
-

User Aids

- Building and Searching Structures on STN
 - Online Helps (HELP DIRECTORY lists all help messages available)
 - STNGUIDE
-

Clusters

- CASRNS
 - NUMERIC
 - STRUCTURE
- [STN Database Clusters](#) information (PDF).
-

Pricing

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

FACTUAL SEARCHING

Search and Display Field Codes

There are no fields that allow left truncation.

Substance Identifying Information

Search Field Name	Search Code	Search Examples	Display Codes
Basic Index (contains single 'words' from ADSM.PA (1), ADSM.PAAN, ASSM.PA (1), ASSM.PAAN, AUN, AZE.PA (1), AZE.PAAN, BPR, AN, BSPM.PA (1), BSPM.PAAN, CDER (1), CDER.AN, CN (1), COMPAN, COMPN (1), CPEM.PA (1), CPEM.PAAN, EDM.PA (1), EDM.PAAN, ENEM.PA (1), ENEM.PAAN, FAN, FMF, HHDG.AN, HHDG.CN (1), INP (1), LLSM.PA (1), LLSM.PAAN, LSSM.PA (1), LSSM.PAAN, LVSM.PA (1), LVSM.PAAN, MECM.PA (1), MECM.PAAN, MF, ODB.PA (1), ODM.PAAN, POT.PAN, POT.PRO (1), RN, RSTR.PA (1), RSTR.PAAN, TRAM.PA (1), TRAM.PAAN, SOLM.PA (1), SOLM.PAAN, XREF.CN (1), and all 'Code.KW' fields)	None or /BI	S ETHYL	ADSM, ASSM, AUN, AZE, BPR, AN, BSPM, CDER, CN, COMPAN, COMPN, CPEM, EDM, ENEM, FAN, FMF, HHDG, INP, LLSM, LSSM, LVSM, MECH, MF, ODM, POT, RSTR, TRAM, RN, STR, SOLM, XREF, CODE (2)
Basic Index Pharmacological and Ecological Data (contains all fields from PED data: BIO, BIOD, COEV, ECDH, ECDP, ECTD, ECTOX, EOD, EXCA, PHARM, USC) Accession Number All Keywords Basic Preferred Registry Number CAS Registry Number Chemical Name (1) Chemical Name Segment (1) Composition: Comp. AN (3) Composition: Comp. Name Compound Type Constitution ID (3) Data Entry Date Data Update Date Element Count (specific) (3) Element Ratio Element Symbol	/BIPED /AN /AKW /BPR /RN /CN /CNS /COMPAN /COMPN /CTYPE /CONSID /DED /DUPD /ELEMENT SYMBOL /ELR.XX /ELS	S (AQUA? TOX?)/BIPED S 1915876/AN S CHEMICAL SHIFTS/AKW S 106-24-1/BPR S 100-03-8/RN S CHOLESTEROL/CN S CHOLESTERYL/CNS S 5811/COMPAN S POLYVINYLPYRROLIDONE /COMPN S ETHYLENE/CNS AND POLYMER?/CTYPE S 1003/CONSID S 1990?/DED S 2000/10/24/DUPD S 5/CL S 2/ELR.HC AND 0.5/ELR.OC S O/ELS AND SE/ELS	BIO, BIOD, BPSM, COEV, ECDH, ECDP, ECTD, ECTOX, EOD, EXCA, PHARM, USC AN all display codes for Code.KW fields BPR RN CN, AUN (4) CN COMPAN COMPN CTYPE CONSID DED DUPD MF MF MF

Search and Display Field Codes

Substance Identifying Information (cont'd)

Search Field Name	Search Code	Search Examples	Display Codes
Field Availability (5) Field Not Availability File Segment Formula Weight (3)	/FA /FNA /FS /FW (or /MW)	S ISOELECTRIC POINT/FA S ALCOHOL/CNS AND BP/FNA S STEREO COMPOUND/FS S 3000<FW	FA (6) not displayed FS FW
Fragment AN (3) Fragment Molecular Formula Handbook Citation Lawson Number (3) Linearized Structure Formula Molecular Formula Number of Atoms (3) Number of Elements (3) Number of Fragments (3) Periodic Group Property Hierarchy (7) STN Update Date (3) Structure Image	/FAN /FMF /HSO /LN /LSF /MF /ATC /ELC /NF /PG /PH /UP	S 1073/FAN S C6H12O6/FMF S 3-01-00-00034/HSO S 22/LN S "CH2O(1+)"/LSF S C4H9N5.H3O4P/MF S 34-36/ATC S 5/C AND 5/ELC S 3/NF S (A3 AND A6)/PG S MASS SPECTRUM/PH S L1 AND 20020701-20020731/UP STR 1209246	FAN FMF HSO LN LSF MF MF FMF, MF MF not displayed not displayed

(1) Input partly in German.

(2) All codes with keywords.

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

(4) The CN display field contains, if available, the Chemical Name (CN) and the AUTONOM Name (AUN).

(5) Searching for all information available for each display field.

(6) DISPLAY FA shows all display field codes available for a record.

(7) Displayed with related properties.

Search and Display Field Codes

Bibliographic Information

Search Field Name	Search Code	Search Examples	Display Codes
Author (1) BABS Accession Number Citation (unresolved) Document Type (1) International Standard (Document) Number (CODEN) Journal Title (1) Journal/Review without CODEN	/AU /BABSAN /URES /DT /ISN /JT /JTW	S SHARPLESS?/AU S 5500103/BABSAN S PERKIN?/URES S PATENT/DT S JACSAT/ISN S TETRAHEDRON/JT S "JOURNAL OF THE SOCIETY OF DYERS AND COLOURISTS"/JTW	(2) BABSAN (2) not displayed (2)
Language (code and text) Patent Assignee (1) Patent Country Patent Number (1) Publication Year (1,3)	/LA /PA /PC /PN /PY	S JA/LA S BASF/PA S US/PC S DE 670683/PN S JACSAT/ISN AND 2000/PY	not displayed (2) (2) (2) (2)

(1) To restrict search to bibliographic information in substance documents, append .SUB to the search field code, e.g., /JT.SUB. To restrict search to reaction data, append .RX to the search field code, e.g., /AU.RX.

(2) References are included in the field containing search term. References may contain a connection to BABS in the form of: BABSNNNNNN. When accessing ReaxysFile using STN on the Web, this BABS Number is a hyperlink to that reference in BABS. Simply click the number.

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

Search and Display Field Codes

Super Search Fields (1)

Search Field Name	Search Code	Fields Searched	Search Examples	Display Codes
All Journal Titles (incl. titles in JT, JTW, and URES)	/AJT	/JT, /JTW, /URES	S IMMUNOCHEMISTRY/AJT	(2)
All Record Numbers	/AAN	/AN, /COMPAN, /FAN, /AZE.AN, /CPEM.PAAN /ENEM.PAAN /EDM.PAAN, /BSPM.PAAN /ADSM.PAAN /ASSM.PAAN /LVSM.PAAN /LLSM.PAAN /LSSM.PAAN /MECM.PAAN /TRAM.PAAN /ODM.PAAN, /RSTR.PAAN /HHDG.AN, /POT.PAN, /CDER.AN, /PHARM.AN, /ECTOX.AN, /BIOD.AN, /ECDH.AN, /ECDP.AN		ADSM, ASSM, AZE, BIOD, AN, BSPM, CDER, COMPAN, CPEM, ECDH, ECDP, ECTOX, EDM, ENEM, FAN, HHDG, LLSM, LSSM, LVSM, MECM, ODM, PHARM, POT, RSTR, SOLM, TRAM
Reaction	/RX	/RX.RCT, /RX.RGT, /RX.PRO, /RX.SUBJ, /RX.SOL, /RX.CAT, /RX.TYP, /RX.PRT, /RX.SRCT	S (ACETIC ACID)/RX	RX

- (1) Enter a super search code to execute a search in one or more fields that may contain the desired information. Super search fields facilitate crossfile and multifile searching. EXPAND may not be used with super search fields. Use EXPAND with the individual field codes instead.
- (2) References are included in the field containing searched term. References may contain a connection to Bibliographies and Abstracts of the ReaxysFile (BABS) in the form of: BABSNNNNNN. When accessing ReaxysFile using STN on the Web, this BABS Number is a hyperlink to that reference in BABS. Simply click the number.

Search and Display Field Codes

Chemical Data

Search Field Name	Search Code	Search Examples	Display Codes
Chemical Derivative Derivative (1) Derivative AN (2) Derivative Comment (1) Isolation from Natural Product (1) Comment (1) Purification (method) (1) Related Structure (1) Comment (1) Referenced Compound (1) Referenced AN (2)	/CDER /CDER.AN /CDER.COM /INP /INP.COM /PUR /RSTR /RSTR.COM /RSTR.PA /RSTR.PAAN	S 8116437/AN AND HYDRAZONE/CDER S 5845535/CDER.AN S BENZIMIDAZOLE/CDER.COM S LEAVES/INP S DEXTROROTATORY/INP.COM S ALCOHOL/CNS AND ACETYLATION/PUR S CONSTITUTION/RSTR S HANDBOOK/RSTR.COM S OESTRADIOLDIMETHYLEETHER/RSTR.PA S 1581/RSTR.PAAN	CDER CDER CDER INP INP PUR RSTR RSTR RSTR RSTR
Crossfile Reference Data Type External Access ID Name (1) Other Source	/XREF.DTP /XREF.ID /XREF.CN /XREF.SO (or /OS)	S 6279685/AN AND IR/XREF.DTP S ALDRICH/XREF.SO(P)250619/XREF.ID S N-BENZOYL-4-PIPERIDONE/XREF.CN S MERCK INDEX/OS	XREF XREF XREF XREF

(1) Input partly in German.

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

Reaction Data

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Reaction Basic Index (contains single words from RX.CAT, RX.CL, RX.COM, RX.COND, RX.PAN, RX.PRO, RX.RAN, RX.RCT, RX.RGT, RX.SOL, RX.SRAN, RX.SRCT, RX.SUBJ, RX.TYP)	-	/BIRX	S CONDENSATION/BIRX	RX
Field Availability Reaction	-	/FA.RX	S REACTION DOCUMENTS/FA.RX	not displayed
All AN Reaction (1,2)	-	/RX.AAN	S 50000/RX.AAN	RX
Catalyst (3)	-	/RX.CAT	S SNBR2/RX.CAT	RX
Reaction Classification (3)	-	/RX.CL	S (CHEMICAL(W)BEHAVIOUR)/RX.CL	RX
Comment (3,4)	-	/RX.COM	S (CRYSTALLINE(W)SUBSTANCE)/RX.CO	RX
Other Conditions (3,4)	-	/RX.COND	S ICEWATER/RX.COND	RX
Reaction ID (2)	-	/RX.ID	S 5418675/RX.ID	RX
No. of Reaction Details (2)	-	/RX.NVAR	S 2/RX.NVAR	RX
Pressure (2,3)	Torr	/RX.P	S 1-25/RX.P	RX
Product AN (2)	-	/RX.PAN	S 4885619/RX.PAN	RX
pH Value (2,3)	-	/RX.PH	S RX.PH<1	RX
Product (4)	-	/RX.PRO	S "CHLORPROMAZINE N+- GLUCURONIDE CHLORIDE"/RX.PRO	RX
Prototype Reaction (3)	-	/RX.PRT	S CATALYST?/RX.PRT	RX
Reactant AN (2)	-	/RX.RAN	S 5026/RX.RAN	RX
Reactant (4)	-	/RX.RCT	S L-PROLINE/RX.RCT	RX
Reagent (3,4)	-	/RX.RGT	S ACETONE/RX.RGT	RX
Reaction Details Reaction ID (3)	-	/RX.RID	S 1000.2/RX.RID	RX
Number of Stages (3)	-	/RX.SNR	S 2/RX.SNR	RX
Solvent (3)	-	/RX.SOL	S CH2CL2/RX.SOL	RX
Stage Reactant AN (2,3)	-	/RX.SRAN	S 742586/RX.SRAN	RX
Stage Reactant (3,4)	-	/RX.SRCT	S MALONALDEHYDE/RX.SRCT	RX
Subject Studied (3)	-	/RX.SUBJ	S KINETICS/RX.SUBJ	RX
Temperature (2,3)	Cel	/RX.T	S -100 - -10/RX.T	RX
Time (3)	-	/RX.TIM	S "2.0 HOUR(S)"/RX.TIM	RX
Reaction Type (3)	-	/RX.TYP	S POLYMERIZATION/RX.TYP	RX
Yield (2,3,5)	-	/RX.YD	S 99.99/RX.YD	RX
Yield Data (3,5)	-	/RX.YDT	S "1 G (AN=1864069)"/RX.YDT	RXT

(1) A search in /RX.ABAN includes the parameters: Reactant AN, Product AN and Stage Reactant AN.

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

(3) Reaction Detail: Included in the default display format QRD only when searched for a reaction detail.

(4) Input partly in German.

(5) Values given for yield in the /RX.YD and /RX.YDT are identical but the numeric yield field (/RX.YD) does not exist for all reactions.

Electric and Magnetic Properties

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Dielectric Constant (1)	none	/DIC	S 2-2.2/DIC	DIC
Comment (2)	-	/DIC.COM	S HANDBOOK/DIC.COM	DIC
Frequency (1)	Hz	/DIC.F	S 50000/DIC.F	DIC
Temperature (1)	Cel	/DIC.T	S 20.5/DIC.T	DIC
Electrical Data	-	-	S ELE/FA	ELE
Comment (2)	-	/ELE.COM	S PHENOL/ELE.COM	ELE
Description	-	/ELE.KW	S PIEZOELECTRICITY/ELE.KW	ELE
Magnetic Data	-	-	S MAG/FA	MAG
Comment (2)	-	/MAG.COM	S HANDBOOK/MAG.COM	MAG
Description	-	/MAG.KW	S MAGNETIC MOMENT/MAG.KW	MAG
Magnetic Susceptibility (1)	cm**3/mol*E6	/MSUS	S 0-410/MSUS	MSUS
Comment (2)	-	/MSUS.COM	S RANGE/MSUS.COM	MSUS
Temperature (1)	CEL	/MSUS.T	S 20-25/MSUS.T	
Static Dielectric Constant (1)	none	/DICS	S 2.3-2.301/DICS	DICS
Comment (2)	-	/DICS.COM	S POLARISATION/DICS.COM	DICS
Temperature (1)	Cel	/DICS.T	S DICS.T>20	DICS

(1) Numeric search field that may be searched using numeric operators or ranges.

(2) Input partly in German.

Electrochemical Behaviour

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Dissociation Exponent (pK) (1)	-	/DE	S 1.5-1.55/DE	DE
Comment (2)	-	/DE.COM	S HANDBOOK/DE.COM	DE
Dissociation Group	-	/DE.GRP	S R2NH/DE.GRP	DE
Method	-	/DE.MET	S CONDUCTOMETRIC/DE.MET	DE
Solvent	-	/DE.SOL	S D2O/DE.SOL	DE
Temperature (1)	Cel	/DE.T	S DE.T>180	DE
Type	-	/DE.TYP	S THERMODYNAMIC/DE.TYP	DE
Electrochemical Behaviour	-	-	-	-
Comment (2)	-	/ELCB.COM	S GAS/ELCB.COM	ELCB
Description	-	/ELCB.KW	S PROTON AFFINITY/ELCB.KW	ELCB
Isoelectric Point pH (1)	-	/IEP	S IEP>5.5	IEP
Comment (2)	-	/IEP.COM	S HANDBOOK/IEP.COM	IEP
Solvent	-	/IEP.SOL	S H2O/IEP.SOL	IEP
Electrochemical Characteristics	-	-	-	-
Comment (2)	-	/POT.COM	S CYCLOVOLTAMMETRY/POT.COM	POT
Description	-	/POT.KW	S OXIDATION POTENTIAL/POT.KW	POT
pH-Value (1)	-	/POT.PH	S 1-7/POT.PH	POT
Product	-	/POT.PRO	S PHENYLENEDIAMINE/POT.PRO	POT
Product AN (1)	-	/POT.PAN	S 23241/POT.PAN	POT
Solvent	-	/POT.SOL	S METHANOL/POT.SOL	POT
Temperature (1)	Cel	/POT.T	S POT.T<-10	POT
Cross-Section	-	-	-	-
Comment (2)	-	/XS.COM	S ELEKTRONEN/XS.COM	XS
Description	-	/XS.KW	S COLLISION CROSS-SECTION/XS.KW	XS

(1) Numeric search field that may be searched using numeric operators or ranges.

(2) Input partly in German.

Physical and Mechanical Properties

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Compressibility Comment (1) Description	- -	/CMP.COM /CMP.KW	S HANDBOOK/CMP.COM S ADIABATIC COMPRESSIBILITY/ CMP.KW	CMP CMP
Density of the Liquid (2) Comment (1) Measurement Temperature (2) Reference Temperature (2)	g*cm**3 - Cel Cel	/DEN /DEN.COM /DEN.T /DEN.RT	S 1/DEN S ALCOHOL/DEN.COM S 20/DEN.T S 10/DEN.RT	DEN DEN DEN DEN
Mechanical Property Comment (1) Description	- -	/MEC.COM /MEC.KW	S HANDBOOK/MEC.COM S VISCOSITY/MEC.KW	MEC MEC
Acoustic Property Comment (1) Description	- -	/SOUND.COM /SOUND.KW	S HANDBOOK/SOUND.COM S VELOCITY OF SOUND/SOUND.KW	SOUND SOUND
Surface Tension (2) Comment (1) Temperature (2)	g/s**2 - Cel	/ST /ST.COM /ST.T	S 1.9-2/ST S HANDBOOK/ST.COM S 20-22/ST.T	ST ST ST
Further Information (Physical and Chemical Properties) (3)	-	-	S FINFO/FA	FINFO

(1) Input partly in German.

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

(3) Field contains citations concerning further physical and chemical properties not covered in detail in ReaxysFile. Only available via Field Availability (/FA).

Multi-Component Systems (MCS)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Adsorption (MCS) Comment (1) Description Partner (1) Partner AN (2) Pressure (2) Solvent Temperature (2)	- - - none Torr - Cel	/ADSM.COM /ADSM.KW /ADSM.PA /ADSM.PAAN /ADSM.P /ADSM.SOL /ADSM.T	S HANDBOOK/ADSM.COM S ENTHALPY OF ADSORPTION/ADSM.KW S TRITON X-100/ADSM.PA S 2822009/ADSM.PAAN S 0.5-20/ADSM.P S H2SO4/ADSM.SOL S 100/ADSM.T	ADSM ADSM ADSM ADSM ADSM ADSM ADSM
Association (MCS) Comment (1) Description Partner (1) Partner AN (1) Pressure (2) Solvent Temperature (2)	- - - - Torr - Cel	/ASSM.COM /ASSM.KW /ASSM.PA /ASSM.PAAN /ASSM.P /ASSM.SOL /ASSM.T	S ACIDIC/ASSM.COM S ASSOCIATION WITH COMPOUND/ ASSM.KW S IMIDAZOLE/ASSM.PA S 54438/ASSM.PAAN S 0.5-1.5/ASSM.P S CDCL3/ASSM.SOL S ASSM.T>100	ASSM ASSM ASSM ASSM ASSM ASSM ASSM
Azeotrope (MCS) Azeotrope Partner (1) Azeotropes AN (2) Comment (1) Concentrations Pressure (2) Temperature (2)	- none - - Torr Cel	/AZE.PA /AZE.PAAN /AZE.COM /AZE.C /AZE.P /AZE.T	S DODECANE/AZE.PA S 1697175/AZE.PAAN S HANDBOOK/AZE.COM S 61 MOL-PERCENT/AZE.C S 199.8/AZE.P S 20-25/AZE.T	AZE AZE AZE AZE AZE AZE

Multi-Component Systems (MCS) (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Boundary Surface Phenomena				
Comment (1)	-	/BSPM.COM	S HANDBOOK/BSPM.COM	BSPM
Description	-	/BSPM.KW	S SURFACE TENSION/BSPM.KW	BSPM
Partner (1)	-	/BSPM.PA	S METHANOL/BSPM.PA	BSPM
Partner AN (2)	none	/BSPM.PAAN	S 1098229/BSPM.PAAN	BSPM
Pressure (2)	Torr	/BSPM.P	S 0-750060/BSPM.P	BSPM
Solvent	-	/BSPM.SOL	S H2O/BSPM.SOL	BSPM
Temperature (2)	Cel	/BSPM.T	S 100/BSPM.T	BSPM
Complex Phase Equilibria				
Comment (1)	-	/CPEM.COM	S DEPENDENCE/CPEM.COM	CPEM
Description	-	/CPEM.KW	S PHASE EQUILIBRIUM/CPEM.KW	CPEM
Partner (1)	-	/CPEM.PA	S (NAPHTHALENE AND WATER)/CPEM.PA	CPEM
Partner AN (2)	none	/CPEM.PAAN	S 1421310/CPEM.PAAN	CPEM
Pressure (2)	Torr	/CPEM.P	S 30000-40000/CPEM.P	CPEM
Solvent	-	/CPEM.SOL	S H2O/CPEM.SOL	CPEM
Temperature (2)	Cel	/CPEM.T	S 20/CPEM.T	CPEM
Critical Micelle Concentration (MCS) (2)	g/L	/CMC	S 0.025/CMC	CMC
Comment (1)	-	/CMC.COM	S HANDBOOK/CMC.COM	CMC
Solvent	-	/CMC.SOL	S H2O/CMC.SOL	CMC
Temperature (2)	Cel	/CMC.T	S 0.025/CMC AND 40/CMC.T	CMC
Electrical Data				
Comment (1)	-	/EDM.COM	S CONCENTRATION/EDM.COM	EDM
Description	-	/EDM.KW	S DIELECTRIC CONSTANT/EDM.KW	EDM
Partner (1)	-	/EDM.PA	S TETRATRIACONTAN-1-OL/EDM.PA	EDM
Partner AN (2)	none	/EDM.PAAN	S 1798829/EDM.PAAN	EDM
Temperature (2)	Cel	/EDM.T	S 20-30/EDM.T	EDM
Energy Data (MCS)				
Comment (1)	-	/ENEM.COM	S CYCLOHEXANON/ENEM.COM	ENEM
Description	-	/ENEM.KW	S ENTHALPY OF SOLUTION/ENEM.KW	ENEM
Partner (1)	-	/ENEM.PA	S 1,4-DIOXANE/ENEM.PA	ENEM
Partner AN (2)	-	/ENEM.PAAN	S 969148/ENEM.PAAN	ENEM
Pressure (2)	Torr	/ENEM.P	S 2-20/ENEM.P	ENEM
Solvent	-	/ENEM.SOL	S TOLUENE/ENEM.SOL	ENEM
Temperature (2)	Cel	/ENEM.T	S 25-30/ENEM.T	ENEM
Henry Constant (MCS) (2)	PA*M**3 /mOL	/HNC	S 20-30/HNC	HNC
Comment (1)	-	/HNC.COM	S CONSTANT/HNC.COM	HNC
Log Henry Constant (2)	-	/HNC.LOG	S -5.72/HNC.LOG	HNC
Solvent	-	/HNC.SOL	S H2O/HNC.SOL	HNC
Temperature (2)	Cel	/HNC.T	S 25/HNC.T	HNC
Liquid/Liquid System				
Comment (1)	-	/LLSM.COM	S HANDBOOK/LLSM.COM	LLSM
Description	-	/LLSM.KW	S LIQUID/LIQUID PHASE DIAGRAM/LLSM.KW	LLSM
Partner (1)	-	/LLSM.PA	S TETRACHLOROMETHANE/LLSM.PA	LLSM
Partner AN	-	/LLSM.PAAN	S 1098295/LLSM.PAAN	LLSM
Pressure (2)	Torr	/LLSM.P	S 0-10000/LLSM.P	LLSM
Solvent	-	/LLSM.SOL	S DIMETHYLSULFOXIDE/LLSM.SOL	LLSM
Temperature (2)	Cel	/LLSM.T	S 5-10/LLSM.T	LLSM
Liquid/Solid System				
Comment (1)	-	/LSSM.COM	S HANDBOOK/LSSM.COM	LSSM
Description	-	/LSSM.KW	S PHASE TRANSITION TEMPERATURE?/LSSM.KW	LSSM
Partner (1)	-	/LSSM.PA	S STRYCHNIDIN-10-ONE/LSSM.PA	LSSM
Pressure (2)	Torr	/LSSM.P	S 0-20000/LSSM.P	LSSM
Partner AN (2)	-	/LSSM.PAAN	S 52979/LSSM.PAAN	LSSM

Multi-Component Systems (MCS) (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Solvent Temperature (2) Liquid/Vapour System (MCS)	- Cel	/LSSM.SOL /LSSM.T	S NAPHTHALENE/LSSM.SOL S LSSM.T>200	LSSM LSSM
Comment (1) Description Partner (1) Partner AN (2) Pressure (2) Solvent Temperature (2) Mechanical & Physical Property (MCS)	- - - - Torr - Cel	/LVSM.COM /LVSM.KW /LVSM.PA /LVSM.PAAN /LVSM.P /LVSM.SOL /LVSM.T	S HANDBOOK/LVSM.COM S CRITICAL VOLUME/LVSM.KW S ACETALDEHYDE/LVSM.PA S 506007/LVSM.PAAN S 19000-90000/LVSM.P S PROPAN-1-OL/LVSM.SOL S 120/LVSM.T	LVSM LVSM LVSM LVSM LVSM LVSM LVSM
Comment (1) Description Partner (1) Partner AN (2) Pressure (2) Solvent Temperature Optical Data (MCS)	- - - - Torr - Cel	/MECM.COM /MECM.KW /MECM.PA /MECM.PAAN /MECM.P /MECM.SOL /MECM.T	S DIAGRAM/MECM.COM S ISOTHERMAL COMPRESS?/MECM.KW S OCTAN-1-OL/MECM.PA S 1697461/MECM.PAAN S 1-10/MECM.P S HCL/MECM.SOL S 25-65/MECM.T	MECM MECM MECM MECM MECM MECM MECM
Description Partner (1) Partner AN (2) Partition Constant (Octan-1-o1/Water) (2)	- - - -	/ODM.KW /ODM.PA /ODM.PAAN /POW	S KERR CONSTANT/ODM.KW S PHENOL/ODM.PA S 969616/ODM.PAAN S 1.5-2/POW	ODM ODM ODM POW
log POW (2) Temperature (2) Solubility (MCS) (2)	- Cel g/L	/POW.LOG /POW.T /SLB	S -0.9- -0.7/POW.LOG S 20/POW.T S SLB<0.0001	POW POW SLB
Comment (1) Ratio of Solvents Saturation Solvent Temperature (2) Solubility Product (MCS) (2)	- - - - Cel -	/SLB.COM /SLB.RAT /SLB.SAT /SLB.SOL /SLB.T /SLBP	S PH/SLB.COM S (6 (P) 1)/SLB.RAT S IN PURE SOLVENT/SLB.SAT S DIETHYL ETHER/SLB.SOL S 10/SLB.T S SLBP<0.00002	SLB SLB SLB SLB SLB SLBP
Comment (1) Ratio of Solvents Solvent Temperature (2) Solution Behaviour (MCS)	- - - Cel	/SLBP.COM /SLBP.RAT /SLBP.SOL /SLBP.T	S HANDBOOK/SLBP.COM S (30 (P) PERCENT)/SLBP.RAT S H2O/SLBP.SOL S 25/SLBP.T	SLBP SLBP SLBP SLBP
Comment (1) Description Partner (1) Partner AN (2) Pressure Solvent Temperature (2) Transport Phenomena (MCS)	- - - - Torr - Cel	/SOLM.COM /SOLM.KW /SOLM.PA /SOLM.PAAN /SOLM.P /SOLM.SOL /SOLM.T	S PRESSURE/SOLM.COM S MISCIBILITY/SOLM.KW S XYLITOL/SOLM.PA S 2049713/SOLM.PAAN S 780-850/SOLM.P S TETRAHYDROFURAN/SOLM.SOL S 20/SOLM.T	SOLM SOLM SOLM SOLM SOLM SOLM SOLM
Comment (1) Description Partner (1) Partner AN (2) Pressure (2) Solvent Temperature (2)	- - - - Torr - Cel	/TRAM.COM /TRAM.KW /TRAM.PA /TRAM.PAAN /TRAM.P /TRAM.SOL /TRAM.T	S HANDBOOK/TRAM.COM S DYNAMIC VISCOSITY/TRAM.KW S ETHANOL/TRAM.PA S 1718733/TRAM.PAAN S 0-800000/TRAM.P S PYRIDINE/TRAM.SOL S 9.9/TRAM.T	TRAM TRAM TRAM TRAM TRAM TRAM TRAM

(1) Input partly in German.

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

Optical Properties

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Circular Dichroism				
Comment (1)	-	/CDIC.COM	S HANDBOOK/CDIC.COM	CDIC
Solvent	-	/CDIC.SOL	S CHCL3/CDIC.SOL	CDIC
Mutarotation (2)	deg	/MUT	S 10-20/MUT	MUT
Comment (1)	-	/MUT.COM	S HANDBOOK/MUT.COM	MUT
Concentration	-	/MUT.C	S 0.7 G/100ML/MUT.C	MUT
Length of Path (2)	cm	/MUT.LEN	S MUT.LEN>10	MUT
Solvent	-	/MUT.SOL	S H2O/MUT.SOL	MUT
Temperature (2)	Cel	/MUT.T	S 21/MUT.T	MUT
Time	-	/MUT.TIM	S 1 DAY?/MUT.TIM	MUT
Type	-	/MUT.TYP	S M/MUT.TYP	MUT
Wavelength (2)		/MUT.W	S 589/MUT.W	MUT
Optics				
Comment (1)	-	/OPT.COM	S ACETON/OPT.COM	OPT
Description	-	/OPT.KW	S LINEAR DICHROISM/OPT.KW	OPT
Optical Rotatory Dispersion				
Comment (1)	-	/ORD.COM	S CYCLOHEXANOL/ORD.COM	ORD
Solvent	-	/ORD.SOL	S ETHANOL/ORD.SOL	ORD
Optical Rotatory Power (2)	deg	/ORP	S 39.65-40/ORP	ORP
Comment (1)	-	/ORP.COM	S ACETAMIDE/ORP.COM	ORP
Concentration	-	/ORP.C	S 1 MOL/L/ORP.C	ORP
Length of Path (2)	cm	/ORP.LEN	S 10/ORP.LEN	ORP
Solvent	-	/ORP.SOL	S BENZENE/ORP.SOL	ORP
Temperature (2)	Cel	/ORP.T	S 20/ORP.T	ORP
Type	-	/ORP.TYP	S ALPHA/ORP.TYP	ORP
Wavelength (2)	nm	/ORP.W	S 578/ORP.W	ORP
Refractive Index (2)				
Comment (1)	-	/RI	S 1.00056/RI	RI
Temperature (2)	Cel	/RI.COM	S HANDBOOK/RI.COM	RI
Wavelength (2)	nm	/RI.T	S 0/RI.T	RI
		/RI.W	S 586/RI.W	RI

(1) Input partly in German.

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

Pharmacological and Ecological Data

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
ECOLOGICAL DATA				
Abiotic Degradation, Hydrolysis				
Degradation Product AN (1)	-	/ECDH.AN	S 647116/EDCH.AN	EDCH
Concentration	-	/ECDH.C	S 0.21 PPM/EDCH.C	EDCH
Comment (2)	-	/ECDH.COM	S (FURTHER (W) DEGRADATION (W) PRODUCT?)/EDCH.COM	EDCH
Degradation Rate	-	/EDCH.D	S 100/EDCH.D	EDCH
Degradation Product (2)	-	/EDCH.DP	S OCTACHLORODIBENZOFURAN/EDCH.DP	EDCH
Exposure Period	-	/EDCH.EX	S 24 HOUR?/EDCH.EX	EDCH
Half-life Time	-	/EDCH.H	S 0.533333 – 16.5/EDCH.H	EDCH
Method, Remarks	-	/EDCH.MR	S GC/EDCH.MR	EDCH
pH-Value	-	/EDCH.PH	S 1.01/EDCH.PH	EDCH
Rate Constant	-	/EDCH.RC	S 1.15 PER HOUR/EDCH.RC	EDCH
Temperature	-	/EDCH.T	S 10/EDCH.T	EDCH
Type	-	/EDCH.TYP	S OXIDATION/EDCH.TYP	EDCH

Pharmacological and Ecological Data (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Abiotic Degradation, Photolysis				
Degradation Product AN (1)	-	/ECDP.AN	S 1446588/ECDP.AN	ECDP
Concentration	-	/ECDP.C	S 5.9 PPM/ECDP.C	ECDP
Comment (2)	-	/ECDP.COM	S (DEGRADATION (W) PRODUCT?) /ECDP.COM	ECDP
Degradation Rate	-	/ECDP.D	S 80/ECDP.D	ECDP
Degradation Product (2)	-	/ECDP.DP	S HEXACHLOROETHANE/ECDP.DP	ECDP
Exposure Period	-	/ECDP.EX	S 3 HOUR?/ECDP.EX	ECDP
Half-life Time	-	/ECDP.H	S 1/ECDP.H	ECDP
Method, Remarks	-	/ECDP.MR	S H2O2/ECDP.MR	ECDP
pH-Value	-	/ECDP.PH	S PHOTOOXIDATION/ECDP.TYP (P) 2.8/ECDP.PH	ECDP
Rate Constant	-	/ECDP.RC	S 0.005 - 2.473 min-1/ECDP.RC	ECDP
Temperature	-	/ECDP.T	S 600/ECDP.T	ECDP
Type	-	/ECDP.TYP	S PHOTOLYSIS/ECDP.TYP	ECDP
Biodegradation				
Comment (2)	-	/BIOD.COM	S (FURTHER (W) DEGRADATION (W) PRODUCT)/BIOD.COM	BIOD
Concentration	-	/BIOD.C	S 1 G/L/BIOD.C	BIOD
Degradation Product (2)	-	/BIOD.DP	S (CARBOXYLATED (W) ALIPHATIC (W) ALCOHOL)/BIOD.DP	BIOD
Degradation Product AN	-	/BIOD.AN	S 8697186/BIOD.AN	BIOD
Degradation Rate	-	/BIOD.D	S 28 - 36/BIOD.D	BIOD
Exposure Period	-	/BIOD.EX	S 8 WEEK?/BIOD.EX	BIOD
Half-life Time	-	/BIOD.H	S 40?/BIOD.H	BIOD
Inoculum	-	/BIOD.IN	S (ACTIVATED (W) SLUDGE)/BIOD.IN	BIOD
Method, Remarks	-	/BIOD.MR	S (SEWAGE (W) TREATMENT)/BIOD.MR	BIOD
Temperature	-	/BIOD.T	S 20/BIOD.T	BIOD
Type	-	/BIOD.TYP	S AEROBIC/BIOD.TYP	BIOD
Biological Behaviour				
Accumulation Half-Life Time	-	/BIO.A	S 5 DAY?/BIO.A	BIO
Accumulation Rate Constant	-	/BIO.AR	S 0.882 PER HOUR/BIO.AR	BIO
Bioconcentration Factor (F)	-	/BIO.BC	S 0.03/BIO.BC	BIO
Biomagnification	-	/BIO.MAG	S 20/BIO.MAG	BIO
Biomonitoring	-	/BIO.MON	S LEUKOCYTES/BIO.MON	BIO
Concentration	-	/BIO.C	S 0.03 - 58 .MY.G/L/BIO.C	BIO
Elimination Half-Life Time	-	/BIO.H	S 28 DAY?/BIO.H	BIO
Elimination Rate Constant	-	/BIO.ER	S 1.1 PER DAY/BIO.ER	BIO
Exposure Period	-	/BIO.EX	S 5 DAY?/BIO.EX	BIO
Log BCF	-	/BIO.LOG	S CA. 8.2/BIO.LOG	BIO
Media	-	/BIO.ME	S FOOD/BIO.ME	BIO
Method, Remarks	-	/BIO.MR	S (FISH (W) BRAIN (W) ACETYLCHOLINESTERASE)/BIO.MR	BIO
Species	-	/BIO.SP	S (SALMO (W) SOLAR)/BIO.SP	BIO
Temperature (1)	C	/BIO.T	S 10-15/BIO.T	BIO
Concentration in Environment				
Background Concentration	-	/COEV.BC	S (FAT (W) BASIS)/COEV.BC	COEV
Contamination Concentration	-	/COEV.CC	S 0 - 20.420 MG/KG DRY WT/COEV.CC	COEV
Location	-	/COEV.LO	S LAKE MICHIGAN/COEV.LO	COEV
Media	-	/COEV.ME	S TOLUENE/CN AND SOIL/COEV.ME	COEV
Method, Remarks	-	/COEV.MR	S (FISH? (S) CAPTURE? (S) APRIL (S)1996)/COEV.MR	COEV
Species	-	/COEV.SP	S FISH/COEV.SP	COEV

Pharmacological and Ecological Data (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Ecological Mobility:				
Transport and Distribution				
Media	-	/ECTD.ME	S WATER-AL2O3/ECTD.ME	ECTD
Method, Remarks	-	/ECTD.MR	S (SOLID (W) PHASE (W) EXTRACTION)/ECTD.MR	ECTD
Results	-	/ECTD.RE	S (SORPTION (W) ISOTHERM)/ECTD.RE	ECTD
Type	-	/ECTD.TYP	S ADSORPTION/ECTD.TYP	ECTD
Ecotoxicology				
Comment (2)	-	/ECTOX.COM	S (FURTHER(W)METABOL?)/ECTOX.COM	ECTOX
Concentration	-	/ECTOX.C	S 3 - 10 .MY.G/L/ECTOX.C	ECTOX
Effect	-	/ECTOX.E	S ABSORPTION/ECTOX.E	ECTOX
Endpoint of Effect	-	/ECTOX.EP	S (GROWTH(W)INHIBITION)/ECTOX.EP	ECTOX
Exposure Period	-	/ECTOX.EX	S 10 DAY?/ECTOX.EX	ECTOX
Further Details	-	/ECTOX.FD	S TEQ/ECTOX.FD	ECTOX
Kind of Dosing	-	/ECTOX.KD	S SOIL/ECTOX.KD	ECTOX
Metabolite (2)	-	/ECTOX.META	S 4-METHYL-3,5-DINITRO-ANILINE/ECTOX.META	ECTOX
Metabolite AN (1)	-	/ECTOX.AN	S 2242347/ECTOX.AN	ECTOX
Method	-	/ECTOX.MR	S (CHOICE (W) BIOASSAY)/ECTOX.MR	ECTOX
Results	-	/ECTOX.RE	S (EFFECTS (2W) OVARIES)/ECTOX.RE	ECTOX
Route of Application	-	/ECTOX.RA	S PERORAL/ECTOX.RA	ECTOX
Sex	-	/ECTOX.S	S FEMALE/ECTOX.S	ECTOX
Species or Test-System	-	/ECTOX.SP	S (EISENIA (W) FOETIDA)/ECTOX.SP	
Type	-	/ECTOX.TYP	S LC50/ECTOX.TYP	ECTOX
Value of Type	-	/ECTOX.V	S CA. 0.2 NKAT/MG PROTEIN/ECTOX.V	ECTOX
Exposure Assessment				
Exposure	-	/EXCA.HE	S (DISTRIBUTION(S)WATER)/EXCA.HE	EXCA
Sources	-	/EXCA.SO	S OIL/EXCA.SO	EXCA
Oxygen Demand				
Concentration	-	/EOD.C	S 1.5 G/EOD.C	EOD
Method, Remarks	-	/EOD.MR	S (STANDARD (2W) METHOD?)/EOD.MR	EOD
Oxygen Demand	-	/EOD.D	S 290.7/EOD.D	EOD
Ratio BOD5/COD	-	/EOD.RAT	S 0.98/EOD.RAT	EOD
Related to	-	/EOD.RE	S DOC/EOD.RE	EOD
Type	-	/EOD.TYP	S BOD10/EOD.TYP	EOD
Stability in Soil				
Caution Exchange Rate	-	/ECS.CE	S "11.45 C MOL (P + T) KG-1"/ECS.CE	ECS
Concentration	-	/ECS.C	S 50 MG/KG/ECS.C	ECS
Dissipation	-	/ECS.D	S 33/ECS.D	ECS
Dissipation Time 50	-	/ECS.5	S 1332/ECS.5	ECS
Dissipation Time 90	-	/ECS.9	S 25D/ECS.9	ECS
Exposure Period	-	/ECS.EX	S (64(W)DAY?)/ECS.EX	ECS
Humidity	-	/ECS.HU	S 0.3 - 2.7 PERCENT/ECS.HU	ECS
Method, Remarks	-	/ECS.MR	S (SOIL (2W) HOLIDAY (W) BEACH)/ECS.MR	ECS
Microbial Biomass	-	/ECS.MB	S 9.8E7 CFU/G/ECS.MB	ECS
Organic Carbon	-	/ECS.OC	S (50 (W) PERCENT)/ECS.OC	ECS
pH-Value (1)	-	/ECS.PH	S 2-5/ECS.PH	ECS
Temperature (1)	C	/ECS.T	S 20>/ECS.T	ECS
Type		/ECS.TYP	S (SANDY (W) LOAM)/ECS.TYP	ECS

Pharmacological and Ecological Data (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
PHARMACOLOGICAL DATA				
Concentration	-	/PHARM.C	S 10 MG/KG/PHARM.C	PHARM
Comment (2)	-	/PHARM.COM	S ANTIFUNGAL/PHARM.COM	PHARM
Effect	-	/PHARM.E	S ACUTE TOXICITY ORAL/PHARM.E	PHARM
Endpoint of Effect	-	/PHARM.EP	S (CELL (W) DEATH)/PHARM.EP	PHARM
Exposure Period	-	/PHARM.EX	S YEAR/PHARM.EX	PHARM
Further Details	-	/PHARM.FD	S ELECTROPHYSIOLOGICAL/PHARM.FD	PHARM
Half-life Time	-	/PHARM.H	S "2 HOUR(S)"/PHARM.H	PHARM
Kind of Dosing	-	/PHARM.KD	S DAILY/PHARM.KD	PHARM
Metabolite (2)	-	/PHARM.META	S PYREN-1-OL/PHARM.META	PHARM
Metabolite AN (1)	-	/PHARM.AN	S 8407954/PHARM.AN	PHARM
Method	-	/PHARM.MR	S (IN (W) VITRO)/PHARM.MR	PHARM
Results	-	/PHARM.RE	S (DOSE (W) DEPENDEN? (P) CYTOTOXICITY/PHARM.RE	PHARM
Route of Application	-	/PHARM.RA	S EPICUTANEOUS/PHARM.RA	PHARM
Sex	-	/PHARM.S	S FEMALE/PHARM.S	PHARM
Species or Test-System	-	/PHARM.SP	S BACTERIA/PHARM.SP	PHARM
Type	-	/PHARM.TYP	S BENZENE/CN AND LD50/PHARM.TYP	PHARM
Value of Type	-	/PHARM.V	S EC50/PHARM.TYP (P) 0.1 MG/L/PHARM.V	PHARM
LABORATORY USE AND HANDLING				
Use of Compound				
Comment (2)	-	/USC.COM	S LIGHT/USC.COM	USC
Laboratory Use and Handling (2)	-	/USC.LH	S (POLYMERIC(2W)SURFACTANT)/USC.LH	USC
Use Pattern	-	/USC.PT	S (DETECTION (2W) PENICILLIN (2W) MILK)/USC.PT	USC

(1) Numeric search field that may be searched using numeric operators or ranges.

(2) Input partly in German.

Safety Data

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Flash Point	CEL	/FP.T	S 105/FP.T	FP
Type of Test (1)	-	/FT.TYP	S DIN/FP.TYP	FP

(1) Numeric search field that may be searched using numeric operators or ranges.

Spectroscopic Data

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
ESR Data				
Comment (1)	-	/ESR.COM	S (INORGANIC(P)COMPOUNDS)/ESR.COM	ESR
Coupling Nuclei	-	/ESR.NUI	S 2D/ESR.NUI	ESR
Description	-	/ESR.KW	S SPECTRUM/ESR.KW	ESR
Solvents	-	/ESR.SOL	S CH2CL2/ESR.SOL	ESR
Temperature (2)	Cel	/ESR.T	S 19-20/ESR.T	ESR
Fluorescence				
Comment (1)	-	/FLU.COM	S HANDBOOK/FLU.COM	FLU
Description	-	/FLU.KW	S MAXIMA/FLU.KW	FLU
Solvent	-	/FLU.SOL	S ACETONITRILE/FLU.SOL	FLU
Temperature (2)	Cel	/FLU.T	S 25/FLU.T	FLU
Infrared Spectrum				
Comment (1)	-	/IR.COM	S PH/IR.COM	IR
Description	-	/IR.KW	S FINE STRUCTURE OF IR BANDS/IR.KW	IR
Solvent	-	/IR.SOL	S CHCL3/IR.SOL	IR
Temperature (2)	Cel	/IR.T	S IR.T>50	IR
Luminescence				
Comment (1)	-	/LUM.COM	S (TEMPERATURE(P)DEPENDE?)/LUM.COM	LUM
Description	-	/LUM.KW	S LUMINESCENCE QUENCHING/LUM.KW	LUM
Mass Spectrum				
Comment (1)	-	/MS.COM	S METASTABLE/MS.COM	MS
Description	-	/MS.KW	S FRAGMENTATION PATTERN/MS.KW	MS
Nuclear Magnetic Resonance				
Comment (1)	-	/NMR.COM	S (AMBIENT (P) TEMPERATURE)/NMR.COM	NMR
Coupling Nuclei	-	/NMR.NUI	S (1H and 13C)/NMR.NUI	NMR
Description	-	/NMR.KW	S 2D-NMR/NMR.KW	NMR
Frequency (2)	-	/NMR.F	S 50/NMR.F	NMR
Nucleus	-	/NMR.NUC	S 31P/NMR.NUC	NMR
Solvents	-	/NMR.SOL	S CDCL3/NMR.SOL	NMR
Temperature (2)	Cel	/NMR.T	S 20-22/NMR.T	NMR
Nuclear Quadrupole Resonance				
Comment (1)	-	/NQR.COM	S (NQR (P) ABSORPTION)/NQR.COM	NQR
Description	-	/NQR.KW	S NUCLEAR QUADRUPOLE RESONANCE/NQR.KW	NQR
Nucleus	-	/NQR.NUC	S 35CL/NQR.NUC	NQR
Other Spectroscopic Methods				
Comment (1)	-	/OSM.COM	S SHIFTS/OSM.COM	OSM
Description	-	/OSM.KW	S PHOTOELECTRON SPECTRUM/OSM.KW	OSM
Phosphorescence				
Comment (1)	-	/PHO.COM	S HANDBOOK/PHO.COM	PHO
Description	-	/PHO.KW	S TRIPLET STATE LIFETIME/PHO.KW	PHO
Solvent	-	/PHO.SOL	S ETHANOL/PHO.SOL	PHO
Temperature (2)	Cel	/PHO.T	S 25/PHO.T	PHO
Raman Spectrum				
Comment (1)	-	/RAS.COM	S (GASEOUS (P) MATRIX)/RAS.COM	RAS
Description	-	/RAS.KW	S RAMAN INTENSITIES/RAS.KW	RAS
Solvent	-	/RAS.SOL	S KBR/RAS.SOL	RAS

Spectroscopic Data (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Rotational Spectrum Comment (1) Description	- -	/ROT.COM /ROT.KW	S ROTATIONS DISPERSION/ROT.COM S ROTATIONAL SPECTRUM/ROT.KW	ROT ROT
UV and Visible Spectrum Absorption Maxima (2) Comment (1) Description Ext./Abs. Coef. (2) Solvent	nm - 1/mol* cm	/UVS.AM /UVS.COM /UVS.KW /UVS.EAC /UVS.SOL	S 139-139.1/UVS.AM S (ACIDIC (P) SOLUTION)/UVS.COM S ABSORPTION MAXIMA/UVS.KW S 4.4/UVS.EAC S CYCLOHEXANE/UVS.SOL	UVS UVS UVS UVS UVS

(1) Input partly in German.

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

Structure and Energy Parameters

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Conformation Object of Investigation	-	/CNF.OBJ	S CONFORMER EQUILIBRIUM/CNF.OBJ	CNF
Dipole Moment Comment (1) Description Moment (2) Method Solvent Temperature (1)	- - D - - Cel	/DM.COM /DM.KW /DM /DM.MET /DM.SOL /DM.T	S CONCENTRATION/DM.COM S QUADRUPOLE MOMENT/DM.KW S 1-1.22/DM S DIELECTRIC/DM.MET S CCL4/DM.SOL S 20>DM.T	DM DM DM DM DM DM
Electrical Polarizability Comment (1) Description	- -	/POL.COM /POL.KW	S (TIME (P) DEPENDENCE)/POL.COM S ELECTRON POLARIZATION/POL.KW	POL POL
Electron Binding Comment (1) Description	- -	/CIP.COM /CIP.KW	S (EXCITED (P) STATE)/CIP.COM S ELECTRON AFFINITY/CIP.KW	CIP CIP
Energy Barrier of Conformation (2) Barrier Type Comment (1) Solvent	- - -	/EBC.TYP /EBC.COM /EBC.SOL	S CF3/EBC.TYP S ROTATION/EBC.COM S TOLUENE/EBC.SOL	EBC EBC EBC
Energy of Dissociation (2) Bond Type Comment (1)	J/mol - -	/EDIS /EDIS.TYP /EDIS.COM	S 12000-14000/EDIS S (P (P) H)/EDIS.TYP S DISSOZIATIONSENERGIE/EDIS.COM	EDIS EDIS EDIS
Ionization Potential (2) Comment (1) Method	eV	/IP /IP.COM /IP.MET	S 7-8/IP S VERTICAL/IP.COM S PHOTOIONIZATION/IP.MET	IP IP IP

Structure and Energy Parameters (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Interatomic Distance and Angle Comment (1) Description	- -	/GEO.COM /GEO.KW	S METHOD/GEO.COM S "INTERATOMIC DISTANCES AND ANGLES"/GEO.KW	GEO GEO
Molecular Deformation Comment (1) Description	- -	/DFM.COM /DFM.KW	S ACETONITRIL?/DFM.COM S FORCE CONSTANTS/DFM.KW	DFM DFM

(1) Numeric search field that may be searched using numeric operators or ranges.

(2) Input partly in German.

State of Aggregation

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
CRYSTALS Crystal Phase Comment (2) Description Temperature (1)	- - Cel	/CRYPH.COM /CRYPH.KW /CRYPH.T	S ANISOTROPIC/CRYPH.COM S CRYSTAL STRUCTURE?/CRYPH.KW S 14.85/CRYPH.T	CRYPH CRYPH CRYPH
Crystal Phase Transition Point (1) Change of Modification Comment (2)	- -	/CTP.COM /CTP.COM	S GLASS/CTP.COM S HANDBOOK/CTP.COM	CTP CTP
Crystal Property Description Colour & Other Properties Comment	- -	/CPD /CPD.COM	S GLAS?/CPD S HANDBOOK/CPD.COM	CDP CDP
Crystal Space Group Comment (2)	-	/CSG /CSG.COM	S P212121/CSG S HANDBOOK/CSG.COM	CSG CSG
Crystal System Comment (2)	-	/CSYS /CSYS.COM	S MONOCLINIC/CSYS S (LABILE (P) FORM)/CSYS.COM	CSYS CSYS
Decomposition Point Comment (2) Solvent	Cel - -	/DP /DP.COM /DP.SO	S 0-10/DP S CRYSTALLIZATION/DP.COM S PROPAN-2-OL/DP.SOL	DP DP DP
Density of the Crystal (1) Comment (2) Temperature (1)	g/cm**3 - Cel	/CDEN /CDEN.COM /CDEN.T	S 5-5.1/CDEN S ORTHORHOMBISCH?/CDEN.COM S 293 K/CDEN.T	CDEN CDEN CDEN
Melting Point (1) Comment (2) Solvent	Cel - -	/MP /MP.COM /MP.SOL	S 250-260/MP S DECOMPOSITION/MP.COM S XYLENE/MP.SOL	MP MP MP
Sublimation Point (1) Comment (2) Pressure (1)	Cel - Torr	/SP /SP.COM /SP.P	S SP>=500 S (MELTING (P) FORM)/SP.COM S 1/SP.P	SP SP SP
Triple Point (1) Comment (2)	Cel -	/TP /TP.COM	S 20-21/TP S HANDBOOK/TP.COM	TP TP

Thermodynamic Properties (cont'd)

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Enthalpy of Hydrogenation (1)	J/mol	/HHDG	S 153362/HHDG	HHDG
Comment (2)	-	/HHDG.COM	S HANDBOOK/HHDG.COM	HHDG
Product AN	-	/HHDG.AN	S 2036502/HHDG.AN	HHDG
Product Name (2)	-	/HHDG.CN	S PHENYL-CYCLOOCTANE/HHDG.CN	HHDG
Temperature	Cel	/HHDG.T	S 24.9/HHDG.T	HHDG
Enthalpy of Sublimation (1)	J/mol	/HSUB	S HSUB<40000	HSUB
Comment (2)	-	/HSUB.COM	S HANDBOOK/HSUB.COM	HSUB
Temperature (1)	Cel	/HSUB.T	S 25/HSUB.T	HSUB
Enthalpy of Vaporization (1)	J/mol	/HVAP	S 90000>HVAP	HVAP
Comment (2)	-	/HVAP.COM	S HANDBOOK/HVAP.COM	HVAP
Pressure (1)	Torr	/HVAP.P	S 250>HVAP.P	HVAP
Temperature (1)	Cel	/HVAP.T	S 20-25/HVAP.T	HVAP
Heat Capacity CP (1)	J/(mol*K)	/CP	S 500-501/CP	CP
Comment (2)	-	/CP.COM	S HANDBOOK/CP.COM	CP
Temperature (1)	F	/CP.T	S CP.T>500	CP
Heat Capacity CpO (1)	J/(mol*K)	/CP0	S 200>CP0	CPO
Comment (2)	-	/CP0.COM	S DETERMIN?/CP0.COM	CPO
Temperature (1)	Cel	/CP0.T	S 200-220/CP0.T	CPO
Heat Capacity CV (1)	J/(mol*K)	/CV	S 113/CV	CV
Comment (2)	-	/CV.COM	S HANDBOOK/CV.COM	CV
Temperature (1)	Cel	/CV.T	113/CV.T (P) 25/CP	CV
Other Thermochemical Data				
Comment (2)	-	/OTHE.COM	S HANDBOOK/OTHE.COM	OTHE
Description	-	/OTHE.KW	S HEAT OF COMBUSTION AT CONSTANT VOLUME/OTHE.KW	OTHE

(1) Numeric search field that may be searched using numeric operators or ranges.

(2) Input partly in German.

Transport Phenomena

Search Field Name	Default Units	Fields Searched	Search Examples	Display Codes
Bulk Viscosity (1)	g/cm*s	/BV	S 52-54/BV	BV
Comment (2)	-	/BV.COM	S CONCENTRATION/BV.COM	BV
Temperature (1)	Cel	/BV.T	S 40-60/BV.T	BV
Dynamic Viscosity (1)	g/cm*s	/DV	S 20/DV.T	DV
Comment (2)	-	/DV.COM	S RANGE/DV.COM	DV
Temperature (1)	Cel	/DV.T	S 20/DV.T	DV
Kinematic Viscosity (1)	cm**2/s	/KV	S 1.9988-1.9999/KV	KV
Comment (2)	-	/KV.COM	S HANDBOOK/KV.COM	KV
Temperature (1)	Cel	/KV.T	S 10/KV.T	KV
Self-Diffusion Coefficient (1)	cm**2/s	/SDIF	S SDIF>=25	SDIF
Comment (2)	-	/SDIF.COM	S HANDBOOK/SDIF.COM	SDIF
Temperature (1)	Cel	/SDIF.T	S 100/SDIF.T	SDIF
Transport Data				
Comment (2)	-	/TRAN.COM	S PRESSURE/TRAN.COM	TRAN
Description	-	/TRAN.KW	S THERMAL CONDUCTIVITY/TRAN.KW	TRAN

(1) Numeric search field that may be searched using numeric operators or ranges.

(2) Input partly in German.

DISPLAY and PRINT Formats

Any combination of display fields and formats may be used to display or print answers. Multiple codes must be separated by commas or spaces. The fields are displayed or printed in the order requested. The default format in the ReaxysFile is the dynamic display format QRD (Query Related Data) providing information on identification of Substance (IDE) plus those display fields in which your search terms appear (HIT). Hit-term highlighting is available for the IDE data (AN, HSO, CN, COMPAN, COMPC, COMPN, CONSID, CTYPE, DED, DUPD, FAN, FMF, FS, FW, LN, LSF, MF, RN). Highlighting must be ON during SEARCH in order to use the HIT format.

The ReaxysFile contains more than 120 display field codes. All display codes may be used as valid formats in the DISPLAY and PRINT commands.

DISPLAY OF REACTION DATA

Substance data and reactions are located in different file segments. After searching for a substance or for substance data, three options are available:

1. Show reactions where the substance is the reaction product (RXPRO).
2. Show reactions with the substance acting as a reactant (RXREA).
3. Display all reactions (RX).

After searching for reaction data (/RX.XYZ) use the display code "RX" to show reactions.

Format	Definition	Examples
RXPRO RXREA RX	Reactions with the searched substance as a product Reactions with the searched substance as a reactant Reactions, only available when searched for reaction data	D L4 RXPRO D RXREA 1-2 D RX

See Online Helps for further information.

DISPLAY AND PRINT FORMATS

All predefined formats are listed in a hierarchical order, whereby the indented subformats are included in the previous format.

Format	Content (corresponding DISPLAY FORMAT or FIELD Codes)	Examples
ALL (1) ALLP ALLREF BABSAN CHE (2) CDER INP PUR RSTR RX (3) HIT (4) IDE (2)	All display fields of CHE, IDE, MCS, PED, PHY, RX (lengthy display) All patent references for a compound All references for a compound BABS Accession Number Chemical Data (CDER, INP, PUR, RSTR, XREF) Chemical Derivative (CDER) Isolation from Natural Product (INP) Purification (PUR) Related Structure (RSTR) Reaction (RX) All fields containing HIT terms Identification of Substance (AUN, BPR, AN, HSO, CN, COMPAN, COMPC, COMPN, CONSID, CTYPE, DED, DUPD, FA, FAN, FMF 5), FS, FW, LN, LSF, MF, RN, STR)	DISPLAY ALL D ALLP D ALLREF D BABSAN D CHE L5 1-4 D CDER DIS L5 1-5 INP DIS L4 PUR D L2 1-3 RSTR DIS RX 1-3 D HIT 1-3 DISPLAY L1 IDE

DISPLAY AND PRINT FORMATS (cont'd)

Format	Content (corresponding DISPLAY FORMAT or FIELD Codes)	Examples
MCS (1)	Multi-Component Systems (ADSM, ASSM, BSPM, EDM, ENEM, LLSM, LSSM, LVS, ODM, MECM, TRAM, SOL)	D 1-6 MCS
ADSM	Adsorption (MCS) (ADSM)	DIS ADSM
ASSM	Association (MCS) (ASSM)	DIS ASSM L3 5
BSPM	Boundary Surface Phenomena (MCS) (BSPM)	D L5 BSPM 1-4
EDM	Electrical Data (MCS) (AZE)	DISPLAY EDM
ENEM	Energy Data (MCS) (ENEM)	DIS L5 1 3 5 ENEM
LLSM	Liquid/Liquid System (MCS) (LSSM)	DIS L8 1 2 LSSM
LSSM	Liquid/Solid System (MCS) (LSSM)	
LVS (2)	Liquid/Vapour System Data (MCS) (AZE, CPEM, LVSM)	D LVS
AZE	Azeotropes (MCS) (AZE)	DISPLY AZE L8
CPEM	Complex Phase Equilibria (MCS) (CPEM)	DISPLAY CPEM L7 2 5
LVSM	Liquid Vapour System (MCS) (LVSM)	DIS L7 1-5 LVSM
MECM	Mechanical and Physical Property (MCS) (MECM)	D MECM L3
ODM	Optical Data (MCS) (ODM)	DIS ODM L7 3
TRAM	Transport Phenomena (MCS) (TRAM)	D TRAM
SOL (2)	Solution Behaviour (MCS) (CMC, HNC, POW, SLB, SLBP, SOLM)	DIS SOL
CMC	Critical Micelle Concentration (MCS) (CMC)	DIS CMC L7 1-10
HNC	Henry Constant (MCS) (HNC)	DIS HNC 1-5
POW	Partition Constant (Octan-1-ol/Water) (MCS) (POW)	Print POW
SLB	Solubility (MCS) (SLB)	DIS L4 1-2 SLB
SLBP	Solubility Product (MCS) (SLBP)	DIS SLBP
SOLM	Solution Behaviour (MCS) (SOLM)	DISPLAY SOLM
PED (2)	Pharmacological and Ecological Data (PHARM, ECO, USC)	DISPLAY PED L5
PHARM	Pharmacological Data (PHARM)	DIS L3 PHARM 1-6
ECO (2)	Ecological Data (BIO, BIOD, COEV, ECDH, ECDP, ECS, ECTD, ECTOX, EOD, EXCA)	D ECO
BIO	Biological Behaviour (BIO)	D BIO 1-6
BIOD	Biodegradation (BIOD)	DIS L40 3 BIOD
COEV	Concentration in Environment (COEV)	DISPLAY COEV L23
ECDH	Abiotic Degradation, Hydrolysis (ECDH)	D ECDH L5 3 6
ECDP	Abiotic Degradation, Photolysis (ECDP)	D ECDP L5 3 6
ECS	Stability in Soil (ECS)	D ECS L9
ECTD	Ecological Mobility: Transport and Distribution (ECTD)	DIS ECTD 10
ECTOX	Ecotoxicology (ECTOX)	DIS ECTOX 1 5
EOD	Oxygen Demand (EOD)	DIS EOD
EXCA	Exposure Assessment (EXCA)	D 1-2 EXCA
USC	Laboratory Use and Handling (USC)	D L3 1-5 USC
PHY (1)	Physical Properties (ECB, ELEP, FINFO, MAGP, MECP, OPTP, SAG, SEP, SF, SPE, THE, TRA)	DISPLAY PHY L6 1
ECB (2)	Electrochemical Behaviour (DE, ELCB, IEP, POT, XS)	DIS ECB
DE	Dissociation Exponent (DE)	DIS L8 DE
ECLB	Electrochemical Behaviour Description (ECLB)	D ECLB 5
IEP	Isoelectric Point (IEP)	DIS IEP L9 1-5
POT	Electrochemical Characteristics (POT)	D POT 1 3 7
XS	Cross Section (XS)	DIS L2 XS
ELEP (2)	Electrical Properties (DIC, DICS, ELE)	DISPLAY ELEP
DIC	Dielectric Constant (DIC)	PRINT DIC L9 1-2
DICS	Static Dielectric Constant (DICS)	DIS L3 1-5 DICS
ELE	Electrical Data (ELE)	DIS ELE L6

DISPLAY AND PRINT FORMATS (cont'd)

Format	Content (corresponding DISPLAY FORMAT or FIELD Codes)	Examples
MAGP (2)	Magnetic Properties (MSUS, MAG)	D L3 MAGP
MSUS	Magnetic Susceptibility (MSUS)	DIS MSUS 1-5
MAG	Magnetic Data (MAG)	DIS MAG L3 1 2
MECP (2)	Physical and Mechanical Properties (CMP, DEN, MEC, SOUND, ST)	DIS L9 1-3 MECP
CMP	Compressibility (CMP)	D 1-5 CMP
DEN	Density of the Liquid (DEN)	DIS DEN 1-5
MEC	Mechanical Properties (MEC)	D MEC L8
SOUND	Acoustic Properties (SOUND)	DIS SOUND 1-6
ST	Surface Tension (ST)	PRINT L3 ST
OPTP (2)	Optical Properties (CDIC, OPT, ORD, ORP, MUT, RI)	D OPTP
CDIC	Circular Dichroism (CDIC)	DISPLAY L1 CDIC
OPT	Optics (OPT)	DIS OPT L
ORD	Optical Rotatory Dispersion (ORD)	D L1 ORD
ORP	Optical Rotatory Power (ORP)	D L3 1-4 ORP
MUT	Mutarotation (MUT)	DIS MUT
RI	Refractive Index (RI)	DISPLAY L7 RI
SAG (1)	State of Aggregation (CRY, GAS, LIQ)	DIS SAG L3
CRY	Crystals (CDEN, CPD, CRYPH, CSG, CSYS, CTP, DP, MP, SP, TP)	D L3 1-7 CRY
CDEN	Density of the Crystal (CDEN)	D CDEN 1-3
CPD	Crystal Property Description (CPD)	DIS CPD 1-3
CRYPH	Crystal Phase Description (CRYPH)	PRINT 1-5 CRYPH
CSG	Crystal Space Group (CSG)	DISPLAY CSG
CSYS	Crystal System (CSYS)	D CSYS 1-5
CTP	Crystal Phase Transition Point (CTP)	DIS 1-3 L8 CTP
DP	Decomposition Point (DP)	D 1-5 DP
MP	Melting Point (MP)	DIS MP L3
SP	Sublimation Point (SP)	D SP
TP	Triple Point (TP)	DIS TP 1-5
GAS (2)	Gases (CRD, CRP, CRT, CRV, GP, VP)	DIS GAS 1-3
CRD	Critical Density (CRD)	D CRD
CRP	Critical Pressure (CRP)	D CRP L3
CRT	Critical Temperature (CRT)	DISPLAY CRT L8
CRV	Critical Volume (CRV)	DIS CRV L3 1-5
GP	Gas Phase Description (GP)	DISPLAY L5 GP
VP	Vapour Pressure (VP)	D VP 1-6
LIQ (2)	Liquids (BP, LIQPH, LPTP)	DIS 1-2 LIQ
BP	Boiling Point (BP)	D L3 BP
LIQPH	Liquid Phase Description (LIQPH)	D LIQPH
LPTP	Transition Point of Liquid Modification (LPTP)	D LPTP 1-10
SEP (2)	Structure and Energy Parameter (CIP, CNF, DFM, DM, EBC, EDIS, GEO, IP, POL)	DISPLAY L3 SEP
CIP	Electron Binding (CIP)	DIS CIP 1-3
CNF	Conformation (CNF)	DIS L1 1-2 CNF
DFM	Molecular Deformation (DFM)	DIS DFM
DM	Dipole Moment (DM)	D DM L5
EBC	Energy Barrier of Conformation (EBC)	D L3 EBC
EDIS	Energy of Dissoziation (EDIS)	D L4 1-5 EDIS
GEO	Interatomic Distance and Angle (GEO)	DISPLAY GEO
IP	Ionization Potential (IP)	DIS IP
POL	Electrical Polarizability (POL)	DIS L3 1-3 POL
SF (2)	Safety Data (FP)	DISPLAY SF L8
FP	Flash Point (FP)	D FP 1-10
SPE (1)	Spectroscopic Data (ESR, FLU, IR, LUM, MS, NMR, NQR, OSM, PHO, RAS, ROT, UVS)	DIS L4 SPE 1-4
ESR	ESR Data (ESR)	D ESR L9
FLU	Fluorescence (FLU)	DISPLAY 1-5 FLU
IR	Infrared Spectrum (IR)	DIS IR 1-10

DISPLAY AND PRINT FORMATS (cont'd)

Format	Content (corresponding DISPLAY FORMAT or FIELD Codes)	Examples
LUM	Luminescence (LUM)	D LUM
MS	Mass Spectrum (MS)	DIS MS 5
NMR	Nuclear Magnetic Resonance (NMR)	DISPLAY NMR L1 1
NQR	Nuclear Quadrupole Resonance (NQR)	DIS NQR
OSM	Other Spectroscopic Methods (OSM)	D L5 OSM
PHO	Phosphorescence (PHO)	DIS PHO 1-4
RAS	Raman Spectrum (RAS)	D L12 1-5 RAS
ROT	Rotational Spectrum (ROT)	DIS ROT
UVS	UV and Visible Spectrum (UVS)	DISPLAY L4 1 UVS
THE (2)	Thermodynamic Properties (CP, CPO, CV, HCOM, HFOR, HFUS, HHDG, HPT, HSUB, HVAP, OTHE)	D THE
FINFO	Further Information (FINFO)	DIS L7 1-5 FINFI
CP	Heat Capacity CP (CP)	D L2 CP
CPO	Heat Capacity CPO (CPO)	D CPO
CV	Heat Capacity CV (CV)	DIS L3 CV
HCOM	Enthalpy of Combustion (HCOM)	PRINT L3 HCOM
HFOR	Enthalpy of Formation (HFOR)	D HFOR
HFUS	Enthalpy of Fusion (HFUS)	D HFUS
HHDG	Enthalpy of Hydrogenation (HHDG)	DISPLAY 1-3 HHDG
HPT	Enthalpies of Other Phase Transitions (HPT)	D L8 HPT
HSUB	Enthalpy of Sublimation (HSUB)	PRINT L3 HSUB
HVAP	Enthalpy of Vaporization (HVAP)	D HVAP
OTHE	Other Thermodynamic Data (OTHE)	D OTHE
TRA (2)	Transport Phenomena (BV, DV, KV, SDIF, TRAN)	D TRA 2, 5
BV	Bulk Viscosity (BV)	D L2 BV
DV	Dynamic Viscosity (DV)	D DV L3 1-35
KV	Kinematic Viscosity (KV)	D KV 17
SDIF	Self-diffusion Coefficient (SDIF)	D SDIF L17
TRAN	Transport Data (TRAN)	D L1 TRAN 1-10
QRD (4)	Query Related Data (default: dynamic format IDE, HIT)	D 5 QRD
FA	Field Availability	D FA 1-5

- (1) Please note, that this format may contain data from multiple fee units.
- (2) All separate custom display fields of this predefined format are together charged as one fee unit.
- (3) Use RX to display reactions when searched for reaction data (/RX.XYZ). Use RXPRES, RXREA or RX. (see preceding table) to display reactions after searching for a substance.
- (4) Default: Dynamic display format QRD (Query Related Data) providing information on Identification of Substance (IDE) plus those display fields in which your search terms appear (HIT)
- (5) For compounds consisting of one fragment, FMF is identical with MF and only MF is displayed.

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).

Field Name	Field Code	ANALYZE/ SELECT (1)	SORT
Abiotic Degradation, Hydrolysis; Degradation Product AN	ECDH.AN	Y (2)	N
Abiotic Degradation, Photolysis; Degradation Product AN	ECDP.AN	Y (2)	N
Accession Number	AN	Y	N
Adsorption (MCS), Partner AN	ADSM.PAAN	Y (2)	N
Association (MCS), Partner AN	ASSM.PAAN	Y (2)	N
Azeotropes AN	AZE.PAAN	Y (2)	N
BABS Accession Number	BABSAN	Y (2)	N
Basic Preferred Registry Number	BPR	Y	N
Biodegradation, Degradation Product AN	BIOD.AN	Y (2)	N
Boundary Surface Phenomena (MCS), Partner AN	BSPM.PAAN	Y (2)	N
CAS Registry Number	RN	Y	N
Chemical Derivative AN	CDER.AN	Y (2)	N
Chemical Name	CN	Y	N
Complex Phase Equilibria Partner AN	CPEM.PAAN	Y (2)	N
Composition: Compound AN	COMPAN	Y	N
Ecotoxicology, Metabolite AN	ECTOX.AN	Y (2)	N
Electrical Data, Partner AN	EDM.PAAN	Y (2)	N
Electrochemical Characteristics, Product AN	POT.PAN	Y (2)	N
Energy Data (MCS), Partner AN	ENEM.PAAN	Y (2)	N
Enthalpy of Hydrogenation Product AN	HHDG.AN	Y (2)	N
Fragment AN	FAN	Y	N
Fragment Molecular Formula	FMF	Y	N
Handbook Citation	HSO	Y	N
Lawson Number	LN	Y	N
Linearized Structure Formula	LSF	Y	N
Liquid/Liquid System, Partner AN	LLSM.PAAN	Y	N
Liquid/Solid System, Partner AN	LSSM.PAAN	Y (2)	N
Liquid/Vapour System, Partner AN	LVSM.PAAN	Y (2)	N
Mechanical and Physical Property (MCS), Partner AN	MECM.PAAN	Y (2)	N
Molecular Formula	MF	Y (default)	N
Molecular Weight	MW (FW)	Y	N
Optical Data (MCS), Partner AN	ODM.PAAN	Y	N
Other Source	XREF.SO	Y	N
Patent Number	PN	Y (2)	N
Pharmacological Data, Metabolite AN	PHARM.AN	Y	N
Product AN	RX.PAN	Y	N
Reactant AN	RX.RAN	Y	N
Reaction Solvent	RX.SOL	Y	N
Related Structure Referenced AN	RSTR.PAAN	Y	N
Solution Behaviour, Partner AN	SOLM.PAAN	Y	N
Stage Reactant AN	RX.SRAN	Y	N
STN Update Date	UP	Y (2)	N
Transport Phenomena (MCS), Partner AN	TRAM.PAAN	Y	N

(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 RN.

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

STRUCTURE SEARCHING

Structure Search Terms

Terms (1)	Search Examples
L-numbers of structures built using the STRUCTURE command or uploaded from STN Express (Boolean logic allowed between the L-numbers)	SEARCH L1 FAM SAM SEA L1 AND L2 SSS FUL
L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers)	S L3 OR L4 SSS SAM
L-number of a structure built using the STRUCTURE command or uploaded from STN Express combined with L-numbers of screen sets created using the SCREEN command (Boolean logic allowed between the L-numbers)	S L1 AND L2 NOT L3

(1) The L-number answer set from a structure search may be combined with dictionary or factual terms, e.g. 'S L6 AND AMINO' or 'S L3 AND IR?/FA'.

Types of Structure Searching

Type	Definition	Search Code	Search Examples
Substructure (default)	Search for substances which match the query. Substitution is allowed at all open positions. Additional components may be retrieved	SSS	SEARCH L1 SSS FUL S L2 OR L3 SSS SAM S L7 SSS RAN
Closed Substructure	Search for substances which match the query exactly. Substitution is allowed at positions opened by CONNECT. Additional components may be retrieved.	CSS	SEARCH L1 CSS FUL S L2 OR L3 CSS S L4 NOT L5 CSS RAN
Family	Search for substances which match the query exactly. Additional components may be retrieved.	FAM	S L6 FAM SAM
Exact	Search for substances which match the query exactly.	EXA	SEA L5 EXA FUL

Scopes of Structure Searches

Type	Definition	Search Code	Search Examples
Sample (default)	Search a fixed 5% of the file	SAM	SEARCH L3 EXA SAM S L6 NOT L7 SSS SAM
Full	Search 100% of the file.	FUL	S L5 OR L8 SSS FUL
Range	Search a user-specified portion of the file.	RAN	S L4 RAN=(5471081,) S L3 FAM RAN=(77542, 80001)
Subset Sample	Search a fixed sample of an answer set created by a search in ReaxysFile.	SUB SAM	S L7 CSS SUB=L5 SAM
Subset Range	Search a user-specified portion of an answer set created by a search in ReaxysFile.	SUB RAN	S L3 SUB=L2 RAN=(,72810)
Subset	Search 100% of an answer set created by a search in	SUB FUL	S L8 SUB=L6 FAM FUL

Full	ReaxysFile.		
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DISPLAY and PRINT Formats

Any combination of display fields and formats may be used to display or print answers. Multiple codes must be separated by commas or spaces. The fields are displayed or printed in the order requested

Hit-term highlighting is available for the IDE data (AN, HSO, CN, COMPAN, COMPC, COMPN, CONSID, CTYPE, DED, DUPD, FAN, FMF, FS, FW, LN, LSF, MF, RN). Highlighting must be ON during SEARCH use the HIT format. The ReaxysFile contains more than 120 display field codes. All display field codes may be used as valid formats in the DISPLAY and PRINT commands.

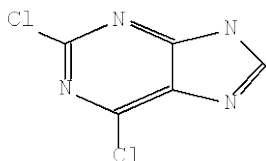
Format (1)	Content	Examples
AN BPR CN, AUN (2) COMPAN COMPC COMPN CONSID CTYPE DED DUPD FA (3) FAN FMF FS FW/MW HSO LN LSF MF RN	Accession Number Basic Preferred Registry Number Chemical Name Composition: Comp. AN Composition: Comp. Conc. Composition: Comp. Name Constitution ID Compound Type Data Entry Date Data Update Date Field Availability Fragment AN Fragment Molecular Formula File Segment Formula Weight Handbook Citation Lawson Number Linearized Structure Formula Molecular Formula CAS Registry Number	D AN DIS BPR L1 1-10 D CN 1 DIS COMPAN D COMPC D L8 2-4 COMPN D CONSID DIS CTYPE D L3 1-5 DED DIS DUPD D FA DIS FAN F1 DISPLAY FMF DISPLAY L1 1- FS D FW DISPLAY L3 BSO DIS LN DISPLAY LSF D MF 1-15 DIS RN 1-5
ALL (4) HIT IDE QRD	All display fields of CHE, IDE, MCS, PED, PHY, RX (lengthy display) All fields containing hit terms Identification of Substance (AUN, BPR, AN, HSO, CN, COMPAN, COMPC, COMPN, CONSID, CTYPE, DED, DUPD, FA, FAN, FMF, FS, FW, LN, LSF, MF, RN, STR) Query Related Data (default: dynamic format IDE, HIT)	DISPLAY ALL D HIT 1-3 DISPLAY L1 IDE D 5 QRD

- (1) In addition to these substance formats, information on Chemical Data (CHE), Substance Identification Data (IDE), Multi-component System data (MCS), Pharmacological and Ecological data (PED), Physical Properties (PHY), and Reactions (RX) are also available, together with references to the primary literature.
- (2) The CN display field contains - if available - the Chemical Name (CN) and the AUTONOM Name (AUN).
- (3) Field Availability search and display field contains an indication of all display fields available in each record (except RN).
- (4) Please note, that this format may contain data from multiple fee units.

Sample Records

DISPLAY IDE

Accession Number (AN): 610966
 Basic Pref. RN (BPR): 5451-40-1
 CAS Reg. No. (RN): 5451-40-1
 Chemical Name (CN): 2,6-dichloro-9H-purine,
 2,6-Dichloropurine,
 2,6-dichloro-7(9)H-purine,
 2,6-dichloro-1H-purine, 2,6-dichloropurine
 Autonom Name (AUN): 2,6-Dichloro-9H-purine
 Lin. Struct. Formula (LSF): C2NHCHNCNCNCl2
 Molec. Formula (MF): C5 H2 Cl2 N4
 Molecular Weight (MW): 189.004
 Compound Type (CTYPE): heterocyclic
 Handbook Citation (HSO): 5-26, 6-26
 Entry Date (DED): 1988/11/28
 Update Date (DUPD): 2009/10/23



Field Availability:

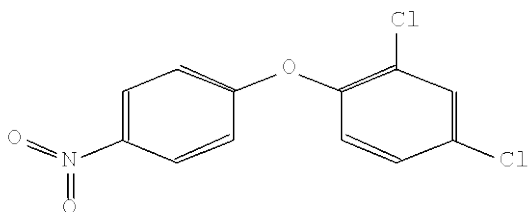
Code	Name	Occurrence
AN	Accession Number	1
BRP	Basic Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	5
AUN	Autonomname	1
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formular Weight	1
CTYPE	Compound Type	1
HSO	Handbook Citation	2
DED	Entry Date	1
DUPD	Update Date	1
DE	Dissociation Exponent	2
ELCB	Electrochemical Behaviour	1
FINFO	Further Information	1
MP	Melting Point	3
MS	Mass Spectrum	1
NMR	Nuclear Magnetic Resonance	5
PHARM	Pharmacological Data	2
UVS	UV and Visible Spectrum	2
XREF	Crossfile Reference	2

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	306
RXREA	Substance is Reaction Reactant	303
RXPRO	Substance is Reaction Product	3

DISPLAY QRD

Accession Number (AN): 1887356
 Basic Pref. RN (BPR): 1836-75-5
 CAS Reg. No. (RN): 1836-75-5
 Chemical Name (CN): Chlomethoxyfen, Nitrofen, NIP,
 2,4-Dichlorophenyl 3-methoxy-4-nitrophenyl
 ether, 2,4-dichlorophenyl-4'-nitrophenyl
 ether, 2,4-dichlorophenyl 4-nitrophenyl
 ether, 2,4-Dichloro-4'-nitrodiphenyl ether
 Autonom Name (AUN): 2,4-Dichloro-1-(4-nitro-phenoxy)-benzene
 Lin. Struct. Formula (LSF): C12H7Cl2NO3
 Molec. Formula (MF): C12 H7 Cl2 N O3
 Molecular Weight (MW): 284.098
 Compound Type (CTYPE): isocyclic
 Handbook Citation (HSO): 5-06, 3-06-00-00821, 4-06-00-01288, 6-06
 Entry Date (DED): 1989/06/29
 Update Date (DUPD): 2009/06/20



Field Availability:

Code	Name	Occurrence
AN	Accession Number	1
BRP	Basic Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	7
AUN	Autonomname	1
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formular Weight	1
CTYPE	Compound Type	1
HSO	Handbook Citation	4
DED	Entry Date	1
DUPD	Update Date	1
BIO	Biological Behaviour	1

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BP	Boiling Point	2
COEV	Concentration in Environment	8
CPD	Crystal Property Description	1
ECDH	Abiotic Degradation, Hydrolysis	1
ECS	Stability in Soil	2
ECTD	Ecological Mobility	2
ECTOX	Ecotoxicology	4
FINFO	Further Information	1
HFUS	Enthalpy of Fusion	1
IR	Infrared Spectrum	2
MP	Melting Point	10
MS	Mass Spectrum	1
PHARM	Pharmacological Data	44
POT	Electrochemical Characteristics	1
SLB	Solubility (MCS)	1
USC	Use of Compound	6
UVS	UV and Visible Spectrum	2
XREF	Crossfile Reference	3

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	9
RXREA	Substance is Reaction Reactant	5
RXPRO	Substance is Reaction Product	4

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