

Beilstein Database - Facts

ONTAP® Beilstein Database - Facts (389)

FILE DESCRIPTION

Beilstein Database - Facts is a very comprehensive structure and factual database in organic chemistry. It includes structures and properties for about 9 million heterocyclic, acyclic and isocyclic compounds covered in the chemical literature published from 1771 onwards. From 2000 onward, biomolecules, mixtures and polymers are also included.

Companion files to File 390 are **Beilstein Database - Reactions**, File 391, which includes the preparations and chemical reactions of the substances in File 390 and **Beilstein Database - Abstracts**, File 393, which includes the literature citations from which the facts and reactions have been extracted.

SUBJECT COVERAGE

Substances included in **Beilstein Database - Facts** must contain Carbon and may also contain any of the following elements from the Periodic Table:

- Group I: H, Li, Na, K, Rb, CS
- Group II: Mg, Ca, Sr, Ba
- Group III: B
- Group IV: C, Si
- Group V: N, P, As
- Group VI: O, S, Se, Te
- Group VII: F, Cl, Br, I

These organic substances may be pure substances with a structural formula or they may be biomolecules, mixtures, or polymers that may be completely or partially described by names or information about their components.

SOURCES

There are three different data sources for **Beilstein Database - Facts**:

1. The *Beilstein Handbook*, Basic Series through Supplement IV, covering journals, books, and patents from 1771 to 1959. Complete evaluated *Handbook* data with corresponding reference to the original literature.

2. Primary literature, (journals, books, and patents) from 1960 to 1979 that is the basis of the *Beilstein Handbook* Supplement V that is still being prepared and updated to provide data beyond the basic data (melting point, boiling point, density, refractive index, optical rotatory power, isolation from natural products and chemical derivatives) already in the file. All other data is provided as keywords with the corresponding references to the original literature.

3. Primary literature (176 journals) from 1980 forward. Detailed information for all physical properties, chemical properties and pharmacological and ecological data is abstracted with corresponding references to the original literature.

TIPS

USE FILE 390

to find physical properties, structures, or pharmacological and ecological data for organic substances, biomolecules, mixtures, and polymers.

USE (S) PROXIMITY

to precisely search a property value and its measurement conditions.

S BP=100:105(S)BPP=.1.:15

USE (F) PROXIMITY

to search for a property measured under specific conditions.

S DP=IR?(F)SOLVENT=BENZENE

USE MAP BNMAIN

to create a SearchSave of Beilstein Registry Numbers for further searching in the Reactions file, File 391.

MAP BNMAIN S5; B 391; EXS

USE GS UDF (User Defined Format)

to display chemical structures in DialogLink.

T S1/2,GS/1-10

DIALOG FILE DATA

Inclusive Dates: 1771 to the present (File 390)
Selected records (File 389)

Update Frequency: Closed (File 389)
Quarterly approx. 55,000 per update (File 390)

File Size: 9,073,120 substances as of September 2004 (File 390)
58,682 records (File 389)

CONTACT

Beilstein Database - Facts is produced by the Beilstein Institute zur Foerderung der Chemischen Wissenschaften. Questions concerning file content should be directed to:

Dialog
The Knowledge Center
11000 Regency Parkway, Suite 10
Cary, NC 27511

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Toll Free: 800-334-2564
Fax: 919-468-9890
E-Mail: dialogcustomer@thomson.com

SAMPLE RECORD - Data Present Format (FORMAT 2)

Sample Record with Handbook and Literature References

BI, ID, BN=, /MAIN
/CN, CN=, /NA, NA=

/SY, SY=, /NA, NA=
RN=
SO=, VO=
DA=
UP=
MF=, ME=, EC=, /EC

NG=
MW=
LN=
CT=
SC=

TR=
CF

DIALOG(R) File 390: Beilstein Database - Facts
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307407

**thiophosphoric acid O, O'-diethyl ester O'-(4-methyl-2-oxo-2H
-chromen-7-yl) ester**

Synonym: 7-diethoxythiophosphoryloxy-4-methyl-coumarin

CAS RN: 299-45-6*

Beilstein Cit: 4-18-00-00343 5-18 6-18

Beilstein Entry Date: 1988/06/27

Beilstein Update: 2002/01/24

Molecular Formula: C14H17O5PS

Number of fragments: 1

Molecular Wt: 328.32

Lawson Nbr: 18943, 298

Compound Type: heterocyclic

Structure Characteristics:

Tautomer possible

Total No. of Rings: 2

Cross File Reference

Description: Coumarin, 7-hydroxy-4-methyl-, O-ester with
O,O-diethyl phosphorothioate Available: RTECS External Access Id:
GN7525000

Similar Stereo Compounds: Constitution Id (CI=): 295996

Similar Tautomer Compounds: Tautomer Id (BT=): 320232

No. Ref: 11

Data Present:

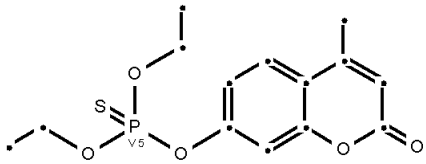
	Data	Refs	Data Type
DPN=	17	2	PP Physical Properties
	12	2	.Physical Properties of Pure Compound
	7		PS ..Physical State
	5		PC ...Crystals
	5		MP ...Melting Point
	2		PL ...Liquids
	2		BP ...Boiling Point
	1		PM ..Other Physical & Mechanical Properties
	1		DN ...Density of the Liquid
	1		OP ..Optics
	1		RI ...Refractive Index
	2	2	SP ..Spectra
	1	1	ES ...Electronic Spectra
	1	1	...Ultraviolet Spectra
	1		EM ...Emission Spectra
	1		...Fluorescence
		1	MS ...Mass Spectrum
	1		EB ..Electrochemical Behavior
	1		...Electrochemical Characteristics
	5		MC ..Physical Properties of Multi-component System
	2		SL ..Solution Behavior
	1		...Solubility
	1		...Partition Constant POW
	3		LL ..Liquid/Liquid System
	3		PE Pharmacological, Ecological, and Use Data
	2		ED ..Ecological Data
	1		ET ..Ecotoxicology
	1		TD ..Transformation and Degradation
	1		AH ...Abiotic Degradation, Hydrolysis
	1		US .Use

SAMPLE RECORD - FORMAT 5 (cont'd)

	acid-((R)-2,3-bis-myristoyloxy-propyl ester)-(2-trimethylammonio-ethyl ester)-betaine, aq. phosphate buffer pH 7.4 Temp: 25 C (Ref. 4)
PE	Pharmacological and Ecological Data
ED	Ecological Data
	Ecotoxicology
/ET,SP=	Effect: pesticidal activity Species or Test-System: Helicoverpa armigera Method: 10 micro lit/pest, solution prepare by dissolving 75 mg of compd. in 10 ml acetone, 12 hr Results: 65 percent mortality (Ref. 6)
TD	Transformation and Degradation
	Abiotic Degradation, Hydrolysis
/AH,TEMP=,PH=	Type: hydrolysis Concentration: 1250 mg/l Temp: Ca. 24 C pH: Ca. 7.3 Method/Remarks: field trial, title comp. accumulated in the cattle dip solution (material containing coumaphos) after incubation in the CFTRL test vat over the period 17 Feb. to 8 June 1993, parathion hydrolase, title comp. content reduced to 427 mg/l (Ref. 11)
US	Laboratory Use and Handling
/US	pesticide (Ref. 4)
RF	References
RF=,BA=,DT=,PA=,PN=	1, 913713 PATENT Farbenfabr. Bayer DE 814297 (1948)(German) DRP/DRBP Org.Chem. ;
AU=,JN=	2, 914001 Schrader Ang. Ch. Monogr. ; 62 (1952)63
CD=	3, 3164320 Ebing CHIMAD ; Chimia ; 21 (1967)132
TI=	4, 6197788 Lopes, Antonio ; Melo, J. Seixas De ; Martins, Armando J. ; Macanita, Antonio L. ; Pina, Fernando S. ; et al. Partition of Pesticides of the Coumarin Family between Water and Amphiphilic Aggregates ESTHAG ; Environ.Sci.Technol. ; 29-3(1995)562 - 570;
TI=	5, 914002 Aldridge ; Davidson BIJOAK ; Biochem.J. ; 52 (1952)663, 669
DT=,TI=	6, 6308156 Chavan, Vishal P. ; Mane, Avinash S. ; Shingare, Murlidhar S. Synthesis of new O,O-dialkyl-O-coumarinophosphorothioates and their pesticidal bioassay against Helicoverpa armigera IJSBDB ; Indian J.Chem.Sect.B ; 40-4(2001)339 - 341;
	7, 914000 BOOK Edwards U.S. Dep. Agric. Bur. Entomol. E-832 (1951)
	8, 3719814 Wasleski JAFCAU ; J.Agric.Food Chem. ; 14 (1966)156
	9, 6266937 Kochansky, Jan Synthesis of (Diethyl-d10) Coumaphos and Related Compounds JAFCAU ; J.Agric.Food Chem. ; 48-7(2000)2826 - 2828;
	10, 913994 Kovac CHZVAN ; Chem.Zvesti ; 8 (1954)272, 276, 277 Chem.Abstr. ; (1955)6784
	11, 6196890 Karns, Jeffrey S. ; Ahrens, Elmer H. ; Davey, Ronald B. ; Shelton, Daniel R. Management of Microbial Processes in Cattle-Dipping Vats Containing Coumaphos PSSCBG ; Pestic.Sci. ; 45-1(1995)13 - 20;

Codes that are not preceded by a slash (/) or followed by an equal sign(=), are display codes, e.g., ID, PC, PL, PM, OP, ES, etc..

SAMPLE RECORD - Chemical Structure*

GR,GS	307407
	Graphic Structure:
	'307407'
	(NA" Tautomer possible",CO"BRN=307407")1P(X293,Y310,V5),2O(X359,Y424),3O(X359,Y197),4O(X163,Y310),5S(X244,Y226),6(X293,Y537),7(X293,Y84),8(X98,Y424),9(X348,Y631),10(X184,Y537),11(X342,Y0),12(X0,Y424),13(X293,Y725),14(X130,Y631),15(X184,Y725),16O(X348,Y819),17(X130,Y819),18(X293,Y914),19(X184,Y914),20(X32,Y819),21O(X342,Y999),2-1-3,4-1=5,6-2,7-3,8-4,9-6=10,11-7,12-8,13=9,14-10,15-13-16,15=14,17-15,18-16,19=17-20,21=18-19.'
structure	 <p>Tautomer possible</p>

* Use GS or GR display code for ROSDAL string that describes structure., or the structure itself, if using DIALOGLINK.

SEARCH OPTIONS

BASIC INDEX

SEARCH SUFFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
—	—	All Basic Index Fields ¹	Segment & Word	S ETHYL S THIOPHOSPHORIC(W)ACID
/AZ	AZ	Azeotrope Component ³	Segment & Word & Phrase	S OL/AZ S ETHANOL/AZ S 1-BUTYLOXY-ETHANOL-(2)/AZ
/CN	CN	Chemical Name ³	Segment & Word & Phrase	S ETHYL/CN S 2H(W)CHROMEN/CN S THIOPHOSPHORIC ACID O, O'-DIETHYL?/CN
/COMMENT	—	Comment	Segment & Word	S AMINO/COMMENT S DECOMPOSITION/COMMENT
/DR	DR	Characterization Derivative ³	Segment & Word & Phrase	S AMINO/DR S DIMETHYL/DR S 2,4-DINITRO-PHENYL?/DR S 2,4-DINITRO-PHENYL?/DR
/EC	MF	Element Count	Word	S C14/EC
/IS	IS	Isolation from Natural Products	Segment & Word & Phrase	S MARITIMA/IS S SCILLA(W)MARITIMA/IS S SCILLA MARITIMA/IS
/NA	NA	Chemical Names and Synonyms ³	Segment & Word & Phrase	S ETHYL/NA S 2H(W)CHROMEN/NA S THIOPHOSPHORIC ACID O, O'-DIETHYL?/NA S ETHYL/NA S 2H(W)CHROMEN/NA S THIOPHOSPHORIC ACID O, O'-DIETHYL?/NA
/PARTNER	—	Partner in a Reported Property ³	Segment & Word & Phrase	S CHLORO/PARTNER S CHLORO(S)METHANE/PARTNER S TRICHLORO-DEUTERIO-METH?/PARTNER S CHLORO/PARTNER(F)DP=TRAM?
—	PR	Purification (display includes IS)	Segment & Word	S CHLORO S TREATMENT(1W)TRIMETHYLCHLOROSILANE
/SOLVENT	—	Solvent	Segment & Word & Phrase	S PHENYL/SOLVENT S AQ(W)PHOSPHATE(W) BUFFER/SOLVENT S AQ. PHOSPHATE BUFFER/SOLVENT
/SY	SY	Synonym	Segment & Word & Phrase	S METHYL/SY S METHYL(W)COUMARIN/SY S 7-DIETHOXYTHIOPHOSPORYLOXY-4?/SY
PHARMACOLOGICAL, ECOLOGICAL, AND USE DATA				
/AH	AH	Abiotic Degradation, Hydrolysis	Segment & Word & Phrase	S THION/AH S PARATHION(W)HYDROLASE/AH S FIELD TRIAL?/AH
/AP	AP	Abiotic Degradation, Photolysis	Segment & Word & Phrase	S CHLORO/AP S TRICHLOROMETHANE/AP S TOC OF TITLE COMP?/AP
/BD	BD	Biodegradation	Segment & Word & Phrase	S CHLORO/BD S TRICHLORO-PYRIDIN?/BD S LAKE MINNETONKA?/BD
/CE	CE	Concentration in the Environment	Segment & Word & Phrase	S CHLORO/CE S DICHLOROMETHANE/CE S VILPPULA, SOUTHERN FINLAND?/CE
—	ED	Ecological Data (Includes ET, EX, MO, TD)	Segment & Word & Phrase	S CHLORO/EE S CHLOROBENZENE/EE S YIELDS OF TITLE COMP?/EE
/EE	EE	Exposure Assessment	Segment & Word & Phrase	S CHLORO/ET S CHLORO/ET S PESTICIDAL(W)ACTIVITY/ET S PESTICIDAL ACTIVITY/ET
/ET	ET	Ecotoxicology	Segment & Word & Phrase	S CHLORO/ET S CHLORO/ET S PESTICIDAL(W)ACTIVITY/ET S PESTICIDAL ACTIVITY/ET
—	EX	Exposure	Segment & Word & Phrase	S CHLORO/MB S DICHLOROACETIC(W)ACID/MB S FISCHER 344 RAT?/MB
/MB	MB	Bioaccumulation, Biomagnification and Biomonitoring	Segment & Word & Phrase	S CHLORO/MB S DICHLOROACETIC(W)ACID/MB S FISCHER 344 RAT?/MB
—	MO	Mobility (Includes MT, MB)	Segment & Word & Phrase	S CHLORO/MT S DICHLOROMETHANE/MT S SEDIMENT?/MT
/MT	MT	Transport and Distribution	Segment & Word & Phrase	S CHLORO/OD S TRICHLOROETHYLENE/OD S ANAEROBIC DECHLORINATION?/OD
/OD	OD	Oxygen Demand	Segment & Word & Phrase	S CHLORO/OD S TRICHLOROETHYLENE/OD S ANAEROBIC DECHLORINATION?/OD
—	PE	Pharmacological, Ecological, and Use Data (Includes PB, ED, and US) ²	Segment & Word & Phrase	S CHLORO/OD S TRICHLOROETHYLENE/OD S ANAEROBIC DECHLORINATION?/OD

BASIC INDEX (cont'd)

SEARCH SUFFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
/PRODUCT	PE	Product (Metabolite or Degradation Product) ³	Segment & Word & Phrase	S PHENYL/PRODUCT S CHLOROPHENYL/PRODUCT S "S-(N- P-CHLOROPHENYL)"?/PRODUCT
/SS	SS	Stability in Soil	Segment & Word & Phrase	S CHLORO/SS S DICHOROACETIC(W)ACID/SS S ARDOYEN SANDY SOIL?/SS
—	TD	Transformation and Degradation (Includes BD, AH, AP, SS, OD)		
/US	US	Use	Segment & Word & Phrase	S AMINO/US S PESTICIDE/US S FLUORIMETRIC DETERMINATION?/US

¹ All words are indexed, including the standard Dialog stop words. Any term in the Basic Index may be limited to a full phrase using /FF, e.g., S PYRIDINE/FF. Any segmented term in the Basic Index may be limited to a full word using /FW, e.g., S PHENOL/FW.

³ Searchable in the Basic Index and in the Additional Indexes.

² Fields in section displayed using main display code (includes pertinent references).

ADDITIONAL INDEXES

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
BASIC INFORMATION ON SUBSTANCE RECORD				
BC=	BC	Component Beilstein Registry Number	Numeric	S BC=1939630
—	BC	Component Data		
—	BI	Basic Information (includes BN, NA, RN, SO, DA, UP, MF,NG or NC and Component Data, MW, LN, SC and Data Present Summary)		
BN=	BN	Beilstein Registry Number ⁴	Numeric	S BN=1896787 S BN=307407/MAIN
CH=	BI	Charge	Numeric	S CH=2
CI=	BI	Constitution ID	Numeric	S CI=295996
CN=	CN	Chemical Name ^{2,3}	Phrase	S CN=THIOPHOSPHORIC ACID O, O'-DIETHYL?
CT=	ID	CompoundType	Phrase	S CT=ACYCLIC S CT=BIOMOLECULE S CT=POLYMER (MONOMERS GIVEN)
EC=	MF	Element Count ³	Phrase	S EC=C0014
GN=	—	Periodic Group Number	Phrase	S GN=A6
—	GS	Graphic Structure		
—	ID	Chemical Identity (same display as BI)		
LF=	BI	Linear Search Form of Molecular Formula	Phrase	S LF="C14H30N2O5(2+)"
LN=	LN	Lawson Number ²	Numeric	S LN=18943
ME=	MF	Molecular Elements	Phrase	S ME=CHOPS
MF=	MF	Molecular Formula	Phrase	S MF=C14H17O5PS
MW=	BI	Molecular Weight (g/mol) ²	Numeric	S MW=328.32
NA=	NA	Chemical Names and Synonyms ³	Phrase	S NA=THIOPHOSPHORIC ACID O, O'-DIETHYL?
NC=	ID	Number of Components	Numeric	S NC=2
NE=	—	Number of Elements	Numeric	S NE=5
PI=	—	Periodic Index Term	Phrase	S PI=A56
PT=	—	Periodic Table Row	Phrase	S PT=T3
RN=	RN	CAS(R) Registry Number	Phrase	S RN=299-45-6
SC=	BI	Structure Characteristics	Phrase	S SC=TAUTOMER POSSIBLE
SO=	SO	Beilstein Source Citation	Phrase	S SO=4-18-00-00343 S SO=4-18 S SO=4
SY=	SY	Synonym ^{2,3}	Phrase	S SY=7-DIETHOXYTHIOPHOSPHORYLOXY-?
TR=	ID	Total Number of Rings	Numeric & Numeric	S TR=4 S TR=2
UD=	—	Update Code	Phrase	S UD=9999
VO=	SO	Beilstein Volume	Phrase	S VO=18
REFERENCES AND DATA PRESENT FIELDS				
AU=	RF	Author	Phrase	S AU=SCHRADER S AU=FARBENFABR. BAYER
BA=	RF	Beilstein Abstract Number of Reference	Phrase	S BA=913713
CD=	RF	CODEN	Phrase	S CD=CHIMAD
—	CF	Cross File References		
DP=	ID	Data Present (Use Format 2)	Phrase	S DP=MP
DPN=	ID	Data Present Name	Phrase	S DPN=MELTING POINT
DT=	RF	Document Type (Reference)	Phrase	S DT=BOOK S DT=PATENT

ADDITIONAL INDEXES (cont'd)

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
HB= JN= NF= NT= PC= PN= RF= — RT= SC=	— RF RF — RF RF — RF — SC	Handbook Data Journal Name Number of References Number of Attributes Patent Country Patent Number Reference Number References Reference Tag Structure Characteristics	Phrase Phrase Numeric Numeric Phrase Phrase Numeric Phrase Phrase	S HB=HANDBOOK(S)DP=MP S JN=PESTIC.SCI. S JN=J.AGRIC.FOOD CHEM. S NF=11 S NT=15 S PC=DE S PN=DE 814297 S RF=9 S RT=FLUORESCENCE QUANTUM YIELD S SC=TAUTOMER POSSIBLE S SC=NO STRUCTURE
PHYSICAL STATE⁵				
BP= BPP= CDN= CPTP= CRDN= CRPRES= CRTEMP= CRVOL= DECOMP= LT= MP= — — — PRES= — SG= SOLVENT= SUB= TEMP= TP= VP= YS=	BP BP PC PC PG PG PG PG PC PL MP PC PG PL PG PS PC — PC PC PC VP PC	Boiling Point (Celsius) Boiling Point Pressure (Torr) Crystal Density (g/cm ³) Transition Point Crystalline Modification Critical Density (g/cm ³) Critical Pressure (Torr) Critical Temperature (Celsius) Critical Volume (cm ³ /mol) Decomposition Point (Celsius) Transition Point Liquid Modification (Celsius) Melting Point (Celsius) Physical Properties of the Crystal Physical Properties of the Gaseous State Physical Properties of the Liquid State Pressure (all values not listed separately) (Torr) Physical Properties of all Physical States ² Crystal Space Group Solvent Sublimation Point (Torr) Temperature (all values not listed separately) (Celsius) Triple Point (Celsius) Vapor Pressure (Torr) Crystal System	Numeric Numeric Numeric Numeric Numeric Numeric Numeric Numeric Numeric Numeric Numeric Word & Phrase Phrase Numeric Numeric Numeric Numeric Numeric Phrase	S BP=108 S BP=210(S)BPP=1 S BPP=760 S CDN=0.8500 S CPTP=17.20 S CRDN=0.2340 S CRPRES=61047.00 S CRTEMP=198.00 S CRVOL=85 S DECOMP=-6 S LT=103.00 S MP=41.5 S PRES=2.00 S SG=C2 S SG="C2 (= C 3 2)" S SOLVENT=PETROLEUM ETHER S SUB=10.00 S TEMP=28.00:38.00 S TP=-183.75 S VP=85.70 S YS=MONOCLINIC
OTHER PHYSICAL and MECHANICAL PROPERTIES⁵				
DN= — ST= TEMP= DI= PARTNER= TEMP= — VB= VD= VK=	PM PM PM — TP TP TP TP TP TP TP	Density (g/cm ³) Other Physical and Mechanical Properties Surface Tension (g/S ²) Temperature (Celsius) Self-Diffusion (cm ² /s) Partner (Transport Phenomena) Temperature (Celsius) Transport Phenomenon data Bulk Viscosity (g/cm ³ *s) Dynamic Viscosity (g/cm ³ *s) Kinematic Viscosity	Numeric Numeric Numeric Numeric Phrase Numeric Numeric Numeric Numeric	S DN=1.26 S ST=26.39 S TEMP=38(S)DN=1.26 S DI=3.0:4.0 S PARTNER=TRICHLORO-DEUTERIO-METH? S TEMP=10:50(F)DP=KV S VB=0.0200 S VD=0.0029 S VK=.3
CALORIFIC DATA⁵				
BN= — CP= CP0= CV= HC= HF= HH= HM= HP= HS= HV= PRODUCT= TEMP=	CA CA CA CA CA CA CA CA CA CA CA CA CA CA	Beilstein Registry Number (Enthalpy of Hydrogenation) Calorific Data Heat Capacity -- cP (J/mol/deg) Heat Capacity -- cP0 (J/mol*deg) Heat Capacity -- cV (J/mol*deg) Enthalpy of Combustion (J/mol) Enthalpy of Formation Enthalpy of Hydrogenation (J/mol) Enthalpy of Melting (J/mol) Other Phase Transition Enthalpies (J/mol) Enthalpy of Sublimation (J/mol) Enthalpy of Vaporization (J/mol) Product (Enthalpy of Hydrogenation) Temperature (Celsius)	Numeric Numeric Numeric Numeric Numeric Numeric Numeric Numeric Numeric Numeric Numeric Phrase Numeric	S BN=3917246(F)DP=HHDG? S BN=3917246/PRODUCT S CP=2.72 S CP0=49.40 S CV=26.84 S HC=-1240800 S HF=-2460500 S HH=-114300 S HM=5198.60 S HP=478.55 S HS=45217.00 S HV=25539.00 S PRODUCT=SUCCINIC ACID? S TEMP=20:25(F)DP=CP
OPTICAL PROPERTIES⁵				

ADDITIONAL INDEXES (cont'd)

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
HN=	SL	Henry Constant (Pa*m3/mol)	Numeric	S HN=2857.1
LH=	SL	Log Henry Constant	Numeric	S LH=3.456
—	LL	Liquid/Liquid Systems ⁶		
—	LS	Liquid/Solid Systems ⁶		
—	LV	Liquid/Vapor Systems (includes Azeotropes) ⁶		
—	MC	Multi-Component Systems Data		
—	OM	Other Multicomponent Data		
PARTNER=	MC	Partner	Phrase	S PARTNER=SULFURIC ACID?
SL=	SL	Solubility (g/l)	Numeric	S SL=.026922
SLP=	SL	Solubility Product	Numeric	S SLP=1.0E-04
SOLVENT=	MC	Solvent	Phrase	S SOLVENT=AQ. PHOSPHATE?(F)DP=SLB
TEMP=	MC	Temperature (Celsius)	Numeric	S TEMP=10:50(F)RT=MELTING DIAGRAM
PHARMACOLOGICAL, ECOLOGICAL, AND USE DATA				
BN=	AH	Beilstein Registry Number (Abiotic Degradation, Hydrolysis Product)	Numeric	S BN=1209246/PRODUCT
BN=	AP	Beilstein Registry Number (Abiotic Degradation, Photolysis Product)	Numeric	S BN=9581893/PRODUCT
BN=	BD	Beilstein Registry Number (Biodegradation Product)	Numeric	S BN=9583513/PRODUCT
BN=	ET	Beilstein Registry Number (Ecotoxicology Metabolite)	Numeric	S BN=9580062/PRODUCT
BN=	PB	Beilstein Registry Number (Pharmacological Data Metabolite)	Numeric	S BN=89402/PB
PH=	AH	pH (Abiotic Degradation, Hydrolysis)	Numeric	S PH=2.14/AH
PH=	AP	pH (Abiotic Degradation, Photolysis)	Numeric	S PH=3/AP
PH=	SS	pH (Stability in Soil)	Numeric	S PH=6.8/SS
PRODUCT=	AH	Product (Abiotic Degradation, Hydrolysis) ³	Phrase	S PRODUCT=FORMIC ACID/AH
PRODUCT=	AP	Product (Abiotic Degradation, Photolysis) ³	Phrase	S PRODUCT=5-AMINO-1-(2,6-DICHLORO?/AP
PRODUCT=	BD	Product (Biodegradation) ³	Phrase	S PRODUCT=N- (4,6-DIMETHOXYPRIMIDIN?/BD
PRODUCT=	ET	Product (Ecotoxicology Metabolite) ³	Phrase	S PRODUCT=VELLOSIMINE/ET
PRODUCT=	PB	Product (Pharmacological Data Metabolite) ³	Phrase	S PRODUCT=LIQUIRITIGENIN/PB
SP=	CE	Species (Concentration in the Environment) ³	Phrase	S SP=HALICHOERUS GRYPUS?/CE
SP=	ET	Species or Test System (Ecotoxicology Data) ³	Phrase	S SP=HELICOVERPA ARMIGERA/ET
SP=	MB	Species (Bioaccum., Magnif, and Biomonitor.) ³	Phrase	S SP=CORBICULA FLUMINEA?/MB
SP=	PB	Species or Test System (Pharmacological Data) ³	Phrase	S SP=C 3H MICE/PB
SX=	ET	Sex (Ecotoxicology Data) ³	Phrase	S SX="MALE AND FEMALE"/ET
SX=	PB	Sex (Pharmacological Data) ³	Phrase	S SX=MALE/PB
TEMP=	AH	Temperature (Celsius) (Abiotic Degradation, Hydrolysis)	Numeric	S TEMP=20:40/AH
TEMP=	AP	Temperature (Celsius) (Abiotic Degradation, Photolysis)	Numeric	S TEMP=50:70/AP
TEMP=	BD	Temperature (Celsius) (Biodegradation)	Numeric	S TEMP=24/BD
TEMP=	MB	Temperature (Celsius) (Bioaccum., Magnif, and Biomonitor.)	Numeric	S TEMP=25/MB
TEMP=	SS	Temperature (Celsius) (Stability in Soil)	Numeric	S TEMP=25/SS
SAFETY DATA⁵				
AT=	SA	Autoignition Temperature	Numeric	S AT=430
FP=	SA	Flash Point (Celsius)	Numeric	S FP=88
—	SA	Safety Data		
STRUCTURE AND ENERGY PARAMETERS⁵				
DM=	SE	Dipole Moment (Debye)	Numeric	S DM=1.92
EBC=	SE	Energy Barriers (J/mol)	Numeric	S EBC=>1000
EDIS=	SE	Dissociation Energy (J/mol)	Numeric	S EDIS=272140
IP=	SE	Ionization Potential (eV)	Numeric	S IP=10.59
—	SE	Structure and Energy Parameters		
DERIVATIVE DATA				
BN=	DR	Beilstein Registry Number (Derivative)	Numeric	S BN=968697/DR
DR=	DR	Characterization Derivative ³	Phrase	S DR=2,4-DINITRO-PHENYLHYDRAZON?
CONSTITUTIONAL DATA				
RC=	SD	Beilstein Registry Number (Related Compound)	Numeric	S RC=1320

⁴ Use /MAIN to restrict a Beilstein Registry Number to the main BN of the record or /OTHER to restrict to other occurrences of the BN in the record.

⁵ All fields in these sections displayable using PP (includes pertinent references).

⁶ For reference or textual data present, search by EXPANDING DPN=field name or RT=field name for comments, e.g., EXPAND RT=LIQUID, RT=EUTECTIC or RT=MELTING DIAGRAM.

Files 390,389
SPECIAL FEATURES

Beilstein Database - Facts

For command descriptions, enter HELP LIMIT, HELP SORT, HELP RANK, HELP MAP online.

LIMIT	<p>/COMMENT -- COMMENT with a reported Property. Apply to subject terms.</p> <p>/ENDPOINT -- Single value or beginning or end value of a range of values. Apply to numerical values that may be reported as ranges.</p> <p>/FW -- Full word; unsegmented.</p> <p>/HIGH -- Single value or high value of a range of values. Apply to numerical values that may be reported as ranges.</p> <p>/LOW -- Single value or low value of a range of values. Apply to numerical values that may be reported as ranges.</p> <p>/MIDPOINT -- Intermediate value in a reported range of values. Apply to numerical values that may be reported as ranges.</p> <p>/PARTNER -- PARTNER in a reported Property. Apply to subject terms or Beilstein Registry Number.</p> <p>/PRODUCT -- PRODUCT, Derivative or Metabolite Apply to subject terms or Beilstein Registry Number.</p> <p>/SOLVENT -- SOLVENT in a reported Property. Apply to a subject term.</p>	<p>S METHYL/COMMENT S S2/COMMENT S TEMP=20/ENDPOINT</p> <p>S BENZENE/FW S TEMP=20/HIGH</p> <p>S TEMP=20/LOW</p> <p>S TEMP=20/MIDPOINT</p> <p>S ETHANOL/PARTNER S BN=969212/PARTNER S S3/PARTNER S PHENYL/PRODUCT S BN=7898025/PRODUCT S S5/PRODUCT S METHANOL/SOLVENT S S1/SOLVENT</p>
SORT	BN, CN, MF	SORT S2/ALL/CN PRINT S4/ALL/MW
RANK	<p>All phrase-indexed and many numeric-indexed fields in the Additional Indexes can be ranked. RANK does not handle well negative numeric values nor values reported as ranges.</p> <p>The following RANK codes are for specific fact groups:</p> <p>BNADSM (Adsorption Partner BN); BNASSM (Association Partner BN); BNAZE (Azeotropes BN); BNBIOD (Bioaccum., Biomagnif., Biomonitor. BN); BNBSPM (Boundry Surface Phenomena BN); BC (Component BN); BNCDER (Derivative BN); BNCPEM (Complex Phase Equilibria Partner BN); BNECDH (Abiotic Degradation, Hydro. Partner BN); BNECDP (Abiotic Degradation, Photo. Partner BN); BNECT (Ecotoxicology Metabolite BN); BNEDM (Electrical Data Partner BN); BNENEM (Energy Data Partner BN); BNHHDG (Enthalpy of Hydrogenation BN); BNLLSM (Liquid/Liquid Systems Partner BN); BNLSSM (Liquid/Solid Systems Partner BN);</p> <p>BNLVSM (Liquid/Vapor Systems Partner BN); BNMECM (Mechanical & Physical Properties Partner BN); BNODM (Optical Data Partner BN); BNPHARM (Pharmacological Data Metabolite BN); BNPOT (Electrochemical Characteristics BN); RC (Referenced Compound BN); BNSOLM (Solution Behaviour Partner BN); BNTRAM (Transport Phenomena Partner BN);</p>	RANK SP
MAP	<p>BA (Beilstein Abstract Number of reference); BN (All BNs in the record); BNMAIN (BN for substance of the record); BNOTHER (BN not found in Main); CN (Chemical Name); NA (Chemical Name and Synonym); PN (Patent Number from references); RN (CAS Registry Number); SY (Synonym - SearchSave for Basic Index search); The following MAP codes are for specific fact groups:</p> <p>BC (Component BN); BNADSM (Adsorption Partner BN); BNASSM (Association Partner BN); BNAZE (Azeotropes BN); BNBIOD (Bioaccum., Biomagnif., Biomonitor. BN); BNBSPM (Boundry Surface Phenomena BN); BNCDER (Derivative BN); BNCPEM (Complex Phase Equilibria Partner BN); BNECDH (Abiotic Degradation, Hydro. Partner BN); BNECDP (Abiotic Degradation, Photo. Partner BN); BNECT (Ecotoxicology Metabolite BN); BNEDM (Electrical Data Partner BN); BNENEM (Energy Data Partner BN); BNHDDG (Enthalpy of Hydrogenation BN); BNLLSM (Liquid/Liquid Systems Partner BN); BNLSSM (Liquid/Solid Systems Partner BN); BNLVSM (Liquid/Vapor Systems Partner BN); BNMECM (Other Mech. & Phys. Prop. in Multi-component Systems Partner BN); BNODM (Optical Data Partner BN); BNPHARM (Pharmacological Data Metabolite BN); BNPOT (Electrochemical Characteristics BN); BNSOLM (Solution Behaviour Partner BN); BNTRAM (Transport Phenomena Partner BN); RC (Related Compound BN);</p>	MAP BNADSM TEMP S2 //MAIN'

PREDEFINED FORMAT OPTIONS

NO.	DIALOGWEB FORMAT	RECORD CONTENT
1	--	DIALOG Accession Number (Beilstein Registry Number)
2	Short	Identification (Beilstein Registry Number, Chemical Name, Molecular Formula, Molecular Weight, Synonym, Number of Fragments, Structure Characteristics, and complete Data Present ⁷)
3	Medium	Identification, Purification, and Isolation from Natural Product Data ⁷
4	--	Identification and Optical Properties ⁷
5	Long	Complete Factual Record (References at end of record) ⁷
6	Free	Molecular Formula, Compound Type, No. of Attributes, No. of References, short Data Present ^{7,8}
7	--	Identification, short Data Present, Pharmacological, Ecological, and Use Data ^{7,8}
8	--	Identification and short Data Present ^{7,8}
9	--	Complete Factual Record (References by section) ⁷
11	--	Format 2 plus References ⁷
15	Full	Full Record including Image (with references after each section) ⁷
K	--	KWIC (Key Word In Context) displays a window of text; may be used alone or with other formats

⁷ Record charges for numbered and user defined formats are by the number of chargeable fields actually present. Presence checking is used to determine the number of chargeable fields in a TYPEd or PRINTed record. Any one chargeable field will show a cost estimate using Format 51. Two chargeable fields will be listed as Format 52, etc. Starting with Format 51, no display code is associated with a format number. These formats are only used in estimating costs for the numbered format or display codes used. See HELP RATES 390 online for actual rates and more details.

⁸ Short Data Present includes only each top line in the hierarchy of any data field, i.e. PR, PP, PE.

OTHER OUTPUT OPTIONS

For an explanation, enter HELP TYPE, HELP UDF, HELP TAG online.

USER DEFINED FORMATS	Display codes listed in the Search Options tables can be used to customize output.	TYPE S2/CN,PP/1-5 TYPE S1/NA,GS/ALL
TAG	Output can be displayed with tags identifying each display field.	TYPE S2/3/ALL TAG
DIRECT RECORD ACCESS	If the accession number of a specific record is known, it can be used to display the record directly.	TYPE 3011556/2 DISPLAY 1999851/ID,GS PRINT 3071746/5

FOR ONLINE HELP:

See HELP FIELDS 390 for searchable fields; HELP FORMAT 390 for output formats; HELP LIMIT 390 for limits; HELP RATES 390 for cost information; HELP SORT 390 for sorts.