

Beilstein Database - Reactions

ONTAP[®] Beilstein Database - Reactions (File 381)

FILE DESCRIPTION

Beilstein Database - Reactions, a companion file to **Beilstein Database - Facts**, File 390, and **Beilstein Database - Abstracts**, File 393, consists of the preparations and chemical reactions associated with the substances in File 390.

SUBJECT COVERAGE

Coverage in **Beilstein Database - Reactions** includes organic reactions classified as:

- Chemical Behaviour
- Chemical Behaviour (Half Reaction)
- Multistage
- Multistage (Half Reaction)
- Preparation
- Preparation (Half Reaction)

Substances for which these reactions are reported 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

SOURCES

Reaction data in **Beilstein Database - Reactions** comes from the following three sources:

1. The *Beilstein Handbook of Organic Chemistry* from the Basic Series to Supplement IV covering the literature from 1771 to 1959. *Handbook* data is available for the reactions of more than 1.1 million compounds.
2. Primary literature (books, journals, patents) published from 1960 to 1979. Reaction data for about 3 million compounds includes reactants, products, reaction classification and references.
3. Primary literature (176 journals) published from 1980 forward. Detailed reaction data is available for the substances reported in these sources. The yearly growth is approximately 220,000 reactions.

TIPS

USE FILE 391

to find the preparation of a specific substance or the chemical reactions in which a specific substance is a reactant or product.

USE /REACTANT

to search a Beilstein Registry Number as a reactant
SELECT BN=109869/REACTANT

USE /PRODUCT

to search a Beilstein Registry Number as a product
SELECT BN=103233/PRODUCT

USE MAP BP

to create a SearchSave of the Beilstein Registry numbers of the products in the reaction for further searching in File 390
MAP BP T; B 390; EXS

USE MAP BR

to create a SearchSave of the Beilstein Registry numbers of the reactants in the reaction for further searching in File 390
MAP BR T; B 390; EXS

DIALOG FILE DATA

Inclusive Dates: 1771 - 2003 (File 381)
1771 to the present (File 391)
Update Frequency: Closed (File 381)
Quarterly Approx. 55,000 reactions (File 391)
File Size: 53,057 records (File 381)
9,510,000 records as of September 2004 (File 391)

CONTACT

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

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Toll Free: 800-334-2564
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Files 391,381
SAMPLE RECORD

Beilstein Database - Reactions

DIALOG(R)File 391:Beilstein Database - Reactions
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ID= Reaction Id: 9178597
BN=, /CN, CN= Reactants
REACTANT= BN=1071742 2-methyl-3-oxo-butyric acid ethyl ester
BN=9259763 6-chloro-2-methylamino-3-nitro-benzonitrile
BN= Products
/CN, CN=, PRODUCT= BN=9278164
2-(2-cyano-3-methylamino-4-nitro-phenyl)-2-methyl-3-oxo-butyric acid ethyl ester
NR= No. of Reaction Details: 3
Reaction Details
CL= Classification: Preparation
YD= Yield: 80 percent (BN=9278164)
REAGENT= Reagent: Cs2CO3
SOLVENT= Solvent: dimethylformamide
TEMP= Temp: 20 C (Ref. 1)
Classification: Chemical behaviour
Reagent: Cs2CO3
Solvent: dimethylformamide
TM= Time: 6 hour(s)
Temp: 20 C
Subject Studied: Product distribution
Prototype Reaction: Further Variations: Reagents Solvents Temperatures (Ref. 1)
Classification: Multistage
Yield: 60 percent (BN=9278164)
NS= No. of Stages: 2
Stage 1:
Reagent: t-BuOK
Solvent: dimethylsulfoxide
Stage 2:
Solvent: dimethylsulfoxide
Time: 1 hour(s)
BN= Reactant BN: 9259763
REACTANT= Reactant: 6-chloro-2-methylamino-3-nitro-benzonitrile (Ref. 2)
RF=, BA=, AU= References
1, 6368675 Snow, Roger J. ; Butz, Tanja ; Hammach, Abdelhakim ; Kapadia, Suresh ; Morwick, Tina M. ; Prokopowicz, Anthony S. ; Takahashi, Hidenori ; Tan, Jonathan D. ; Tschantz, Matt A. ; Wang, Xiao-Jun Isoquinolinone synthesis by S N Ar reaction: a versatile route to imidazo 4,5-h isoquinolin-9-ones TELEAY ; Tetrahedron Lett. ; 43-42(2002)7553 - 7556;
2, 6399906 Goldberg, Daniel R. ; Butz, Tanja ; Cardozo, Mario G. ; Eckner, Robert J. ; Hammach, Abdelhakim ; Huang, Jessica ; Jakes, Scott ; Kapadia, Suresh ; Kashem, Mohammed ; Lukas, Susan ; Morwick, Tina M. ; et al. Optimization of 2-Phenylaminoimidazo 4,5-h isoquinolin-9-ones: Orally Active Inhibitors of lck Kinase JMC MAR ; J.Med.Chem. ; 46-8(2003)1337 - 1349;

SEARCH OPTIONS

BASIC INDEX

SEARCH SUFFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
—	—	All Basic Index Fields ¹	Segment & Word	S AMINO S BUTYRIC(W)ACID
/BP	BP	Chemical Name of Product ²	Segment & Word & Phrase	S AMINO/BP S AMINO(S)NITRO(S)PHENYL/BP
/BR	BR	Chemical Name of Reactant ²	Segment & Word & Phrase	S 2-(2-CYANO-3-METHYLAMINO)?/BP S CHLORO/BR
/CATALYST	RD	Catalyst ²	Segment & Word & Phrase	S CHLORO(S)METHYLAMINO/BR S 6-CHLORO-2-METHYLAMINO?/BR S CHLORO/CATALYST
/CN	BP, BR	Chemical Name ²	Segment & Word & Phrase & Word	S TRIS(W)PHENYLPHOSPHINE/CATALYST S CHLOROTRIS(TRIPHENYL)?/CATALYST S 2-METHYL-3-OXO-BUTYRIC? S BENZONITRILE/CN S BUTYRIC(W)ACID(W)ETHYL(W)ESTER/CN
/COMMENT	RD	Comment	Segment & Word	S CHLORO/COMMENT S OPTICALLY(W)INACTIVE/COMMENT
/PRODUCT	BP	Product ²	Segment & Word & Phrase	S CYANO/PRODUCT S OXO(W)BUTYRIC/PRODUCT S 2-(2-CYANO-3-METHYLAMINO)?/PRODUCT

BASIC INDEX (cont'd)

SEARCH SUFFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
—	RD	Classification ²	Word	S PREPARATION
—	RD	Classification ²	Phrase	S MULTISTAGE (HALF REACTION)
—	RD	Conditions	Segment & Word	S ARYL
—	RD	Conditions	Word	S TRIMETHYL
—	RD	Conditions	Phrase	S MICROWAVE IRRADIATION
—	RD	Prototype Reaction	Word	S SOLVENTS
—	RD	Prototype Reaction	Phrase	S FURTHER(W)VARIATIONS
—	RD	Reaction Type	Word	S FURTHER VARIATIONS?
—	RD	Reaction Type	Phrase	S GRIGNARD
—	RD	Subject Studied	Word	S GRIGNARD ADDITION
—	RD	Subject Studied	Phrase	S PRODUCT(W)DISTRIBUTION
—	RD	Subject Studied	Phrase	S PRODUCT DISTRIBUTION
/REACTANT	BR	Reactant	Segment & Word & Phrase	S NITRO/REACTANT
/REAGENT	RD	Reagent	Segment & Word & Phrase	S OXO(W)BUTYRIC(W)ACID/REACTANT
/SOLVENT	RD	Solvent	Segment & Word & Phrase	S 6-CHLORO-2-METHYL?/REACTANT
				S CS2CO3/REAGENT
				S BUOK/REAGENT
				S T-BUOK/REAGENT
				S SULFOXIDE/SOLVENT
				S METHYL(W)SULFOXIDE/SOLVENT
				S DIMETHYLSULFOXIDE/REAGENT

¹ Chemical substance names are segmented in all Basic Index fields; for example, DICHLOROHEXANE is retrieved when searched as a single term or by searching the segments: DI, CHLORO, HEXANE or CHLOROHEXANE. To exclude the segments use the /FW suffix; e.g., S HEXANE/FW to retrieve the word set off by spaces or punctuation marks.

² Searchable in the Basic Index and in the Additional Indexes.

ADDITIONAL INDEXES

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
AU=	RF	Author	Phrase	S AU=SNOW, ROGER J?
BA=	RF	Beilstein Abstract Id	Numeric	S BA=1071742
BN=	BN	Beilstein Registry Number	Numeric	S BN=1071742
BN=	BP	Beilstein Registry Number of Product	Numeric	S BN=9278164/BP
BN=	BR	Beilstein Registry Number or Reactant	Numeric	S BN=9278164/PRODUCT
BN=	BR	Beilstein Registry Number or Reactant	Numeric	S BN=1071742/BR
CATALYST=	RD	Catalyst	Word & Phrase	S BN=9259763/REACTANT
CD=	RF	CODEN	Phrase	S CATALYST=NI
CL=	RD	Reaction Classification	Phrase	S CATALYST=(RANEY(N)NI)
CN=	BP	Chemical Name of Product	Phrase	S CD=TELEAY
CN=	BR	Chemical Name of Reactant	Phrase	S CL=PREPARATION
CN=	CN	Chemical Name	Phrase	S CN=2-(2-CYANO-3-METHYLAMINO)?/BP
DP=	—	Data Present Code	Phrase	S CN=2-METHYL-3-OXO-BUTYRIC?/BR
DPN=	—	Data Present Name	Phrase	S CN=2-METHYL-3-OXO-BUTYRIC?
DT=	—	Document Type	Phrase	S DP=RX.Y
ID=	ID	Reaction Id	Phrase	S DPN=REACTION YIELD
JN=	RF	Journal Name	Numeric	S DT=PATENT
NF=	—	Number of References	Phrase	S ID=9178597
NR=	—	Number of Reactions	Phrase	S JN=TETRAHEDRON LETT?
NS=	—	Number of Stages	Numeric	S NF=2
PA=	RF	Patent Assignee	Numeric	S NR=3
PC=	RF	Patent Country	Phrase	S NS=2
PH=	RD	pH ³	Phrase	S PA=SYNTEX?
PN=	RF	Patent Number	Phrase	S PC=EP
PRES=	RD	Pressure ³	Numeric	S PH=6.5
PRODUCT=	BP	Product ²	Phrase	S PN=EP 13786
—	RD	Reaction Details	Phrase	S PRES=2
REACTANT=	BR	Reactant ²	Phrase	S PRODUCT=2-(2-CYANO-3-METHYLAMINO)?
REAGENT=	RD	Reagent ²	Phrase	S REACTANT=2-METHYL-3-OXO-BUTYRIC?
RF=	RF	Reference Number	Word & Phrase	S REAGENT=BUOK
SOLVENT=	RD	Solvent ²	Numeric	S REAGENT=T-BUOK
TEMP=	RD	Temperature ³	Word & Phrase	S RF=1
TI=	RF	Title ²	Word & Phrase	S SOLVENT=DIMETHYLSULFOXIDE
TM=	RD	Time	Word & Phrase	S SOLVENT=ACETIC ACID
UD=	—	Update	Phrase	S TEMP=20
				S TI=(INHIBITOR?(2W)KINASE)
				S TI=OPTIMIZATION OF 2-PHENYLAMINO?
				S TM=6
				S TM=6 HOUR?
				S UD=9999

ADDITIONAL INDEXES (cont'd)

SEARCH PREFIX	DISPLAY CODE	FIELD NAME	INDEXING	SELECT EXAMPLES
YD=	RD	Yield (percent)	Numeric	S YD=60

³ Numeric values can be entered in several different ways: directly as a number, i.e., S TEMP=100.0; in exponential notation, i.e., S TEMP=1E2. Letter abbreviations are also available: K for thousand, M for million, B for billion, e.g., S TEMP=0.5K:1.0K. To search a range of values, use a colon between starting and ending values, e.g., S TEMP=75:80, OR use numeric operators (>, <, >=, and <=), e.g., S 75<=TEMP<=80.

SPECIAL FEATURES

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

LIMIT	/ -- DIALOG Accession Number / CATALYST -- CATALYST in Reaction Details. Apply to subject terms. / COMMENT -- COMMENT in Reaction Details. Apply to subject terms. / ENDPOINT -- Single value or beginning or end value of a range of values. Apply to numerical values that may be reported as ranges. / FW -- Full word; unsegmented. / HIGH -- Single value or high value of a range of values. Apply to numerical values that may be reported as ranges. / LOW -- Single value or low value of a range of values. Apply to numerical values that may be reported as ranges. / MIDPOINT -- Intermediate value in a reported range of values. Apply to numerical values that may be reported as ranges. / PRODUCT -- PRODUCT in Reaction Details. Apply to subject terms or Beilstein Registry Number. / REACTANT -- REACTANT in Reaction Details. Apply to subject terms or Beilstein Registry Number. / REAGENT -- REAGENT in Reaction Details. Apply to subject terms. / SOLVENT -- SOLVENT in Reaction Details. Apply to subject terms.	S S1/5000000-9999999 S NI/CATALYST S CHLORO/COMMENT S TEMP=20/ENDPOINT S BENZENE/FW S TEMP=20/HIGH S PRES=.2/LOW S PRES=.1/MIDPOINT S METHYLAMINO/PRODUCT S BN=9278164/PRODUCT S BUTYRIC(W)ACID/REACTANT S BN=9259763/REACTANT S CS2CO3/REAGENT S DIMETHYLFORMAMIDE/SOLVENT
RANK	All phrase- and numeric-indexed fields in the Additional Indexes can be ranked.	RANK REACTANT RANK TM S4
MAP	BA, BN, BP, BR, PN	MAP PN TEMP S2

PREDEFINED FORMAT OPTIONS

NO.	DIALOGWEB FORMAT	RECORD CONTENT
1	--	DIALOG Accession Number
2	--	Reaction Id, Reactants, Products, No. of Reactions, References
3	Medium	Reaction Id, Reactants, Products, No. of Reactions, No. of References
4	--	Full Record
5	--	Full Record
6	Free	Reaction Id, Reactants, Products
7	Long	Full Record
8	Short	Reaction Details
9	Full	Full Record
K	--	KWIC (Key Word In Context) displays a window of text; may be used alone or with other formats

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 S3/BR,BP,RD/ALL
TAG	Output can be displayed with tags identifying each display field.	TYPE S2/5/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 9178597/9 DISPLAY 9036249/RD PRINT 1285/9

FOR ONLINE HELP:

See HELP FIELDS 391 for searchable fields; HELP FORMAT 391 for output formats; HELP LIMIT 391 for limits; HELP RATES 391 for cost information; HELP SORT 391 for sorts.