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中国科学院国家科学图书馆



获取化合物理化性质 及合成制备数据的途径



问题1：如何查找一个科学数据？

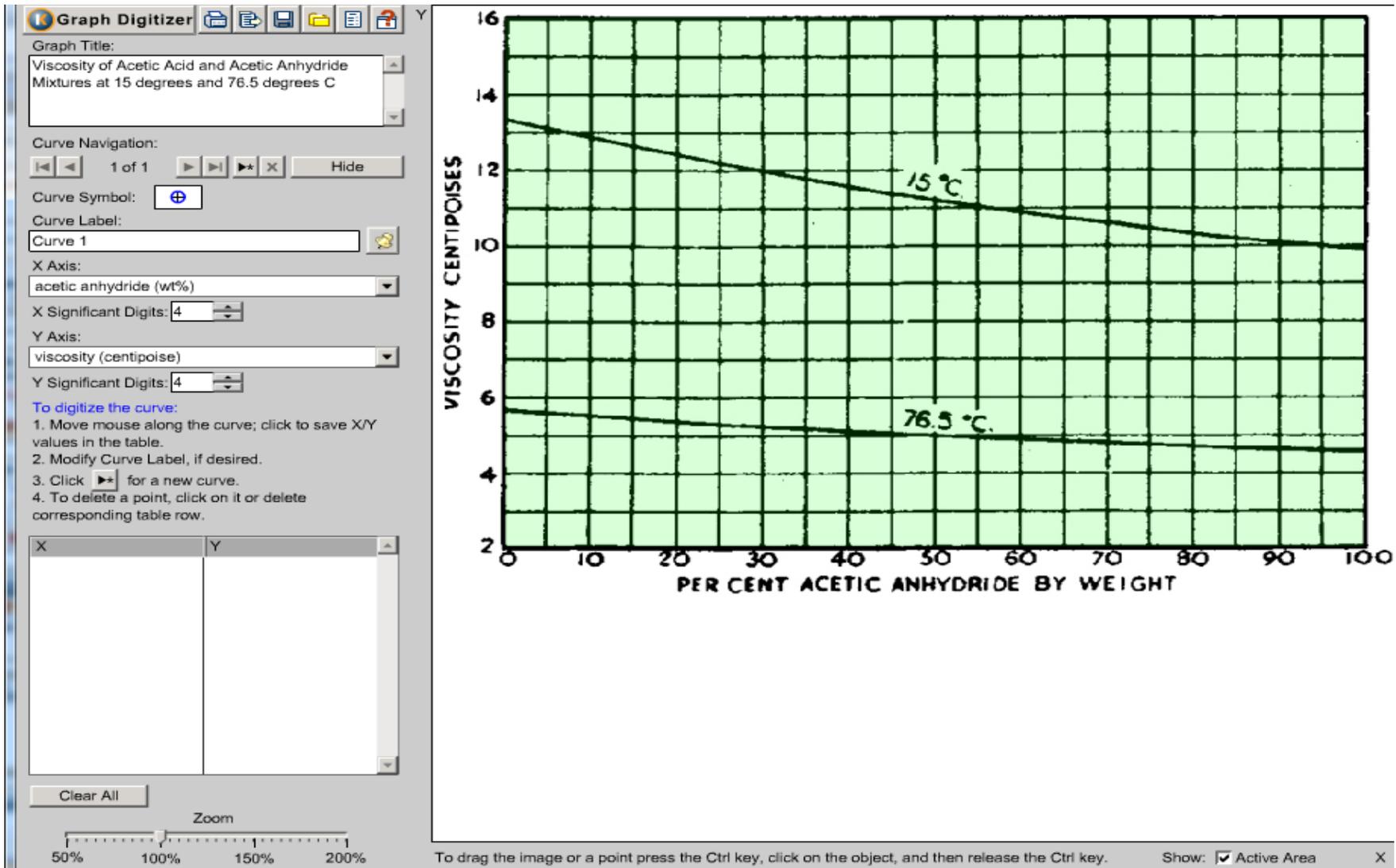
光谱数据
电化学常数
热物理常数
... ..

How do I filter
factual from
speculative
data?





问题2: 如何查找满足现有实验条件的实验数据?



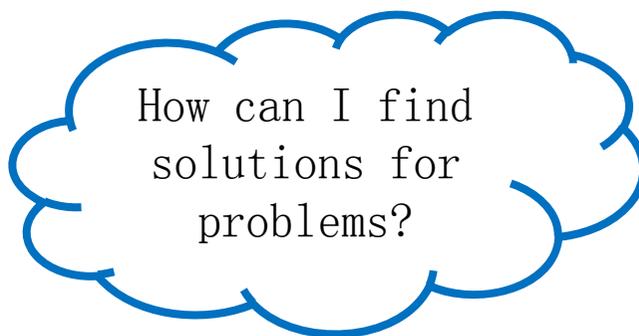


我如何查找国特色类群
知植物图谱？

MPA和KSI单位如何转
换？

如何提高太阳能的转换
效率？

....



一位钢铁厂的冶金学家
收到一个制造要求：

抗张强度至少为415MPa

最大拉伸强度至少为
690MPa的碳钢

符合要求的条件下，碳
钢中碳最佳%...

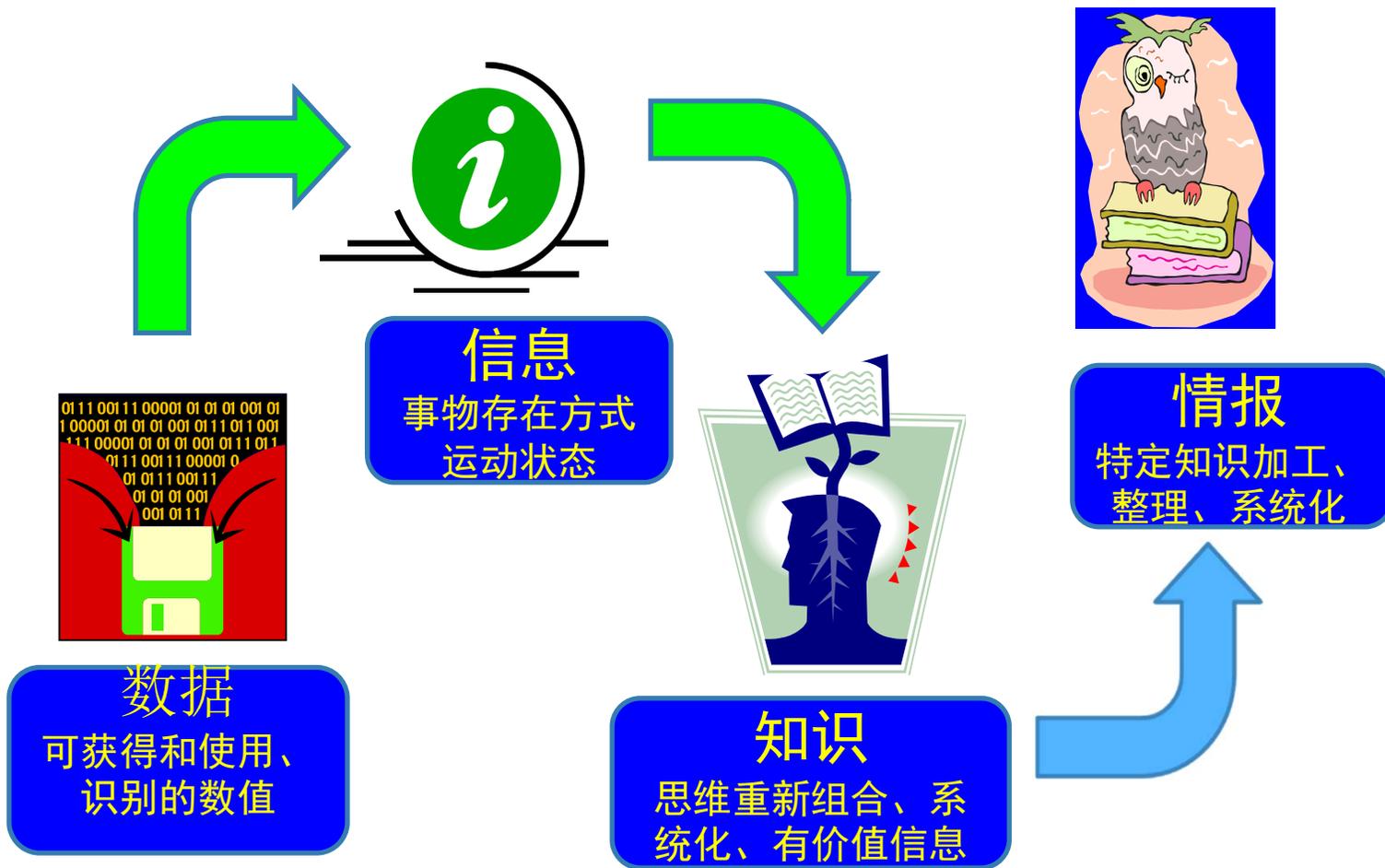


为什么对查找数据会感觉困难



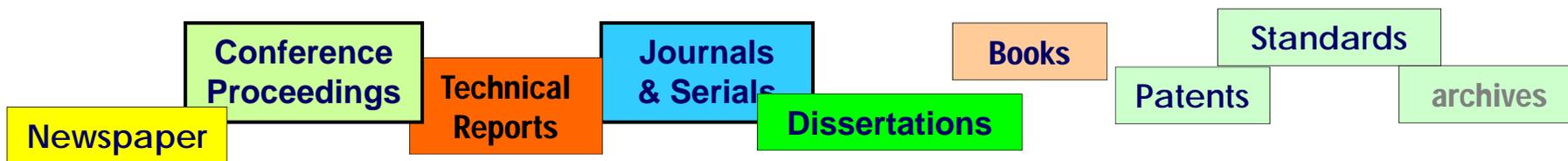
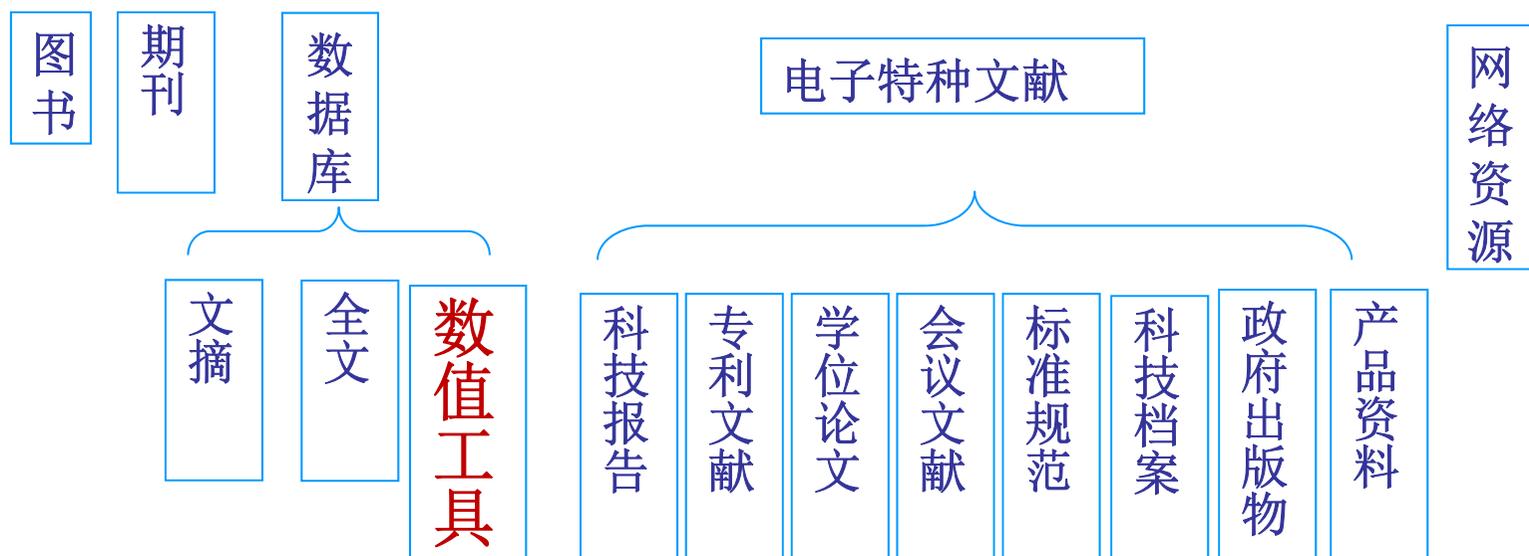


信息相关的概念——丢失了数据





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——Reaxys

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- 实例



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- 包括全部 Landolt Börnstein (LB) 印本资料信息





Landolt Börnstein (LB) 工具书



- Landolt-Börnstein (LB) 工具书由世界著名的科技出版社——德国施普林格出版社(Springer-Verlag) 出版。
- 由Hans Landolt 和 Richard Börnstein两位教授在1883年共同创建了这套工具书，迄今已经有130年历史，是一套连续出版科学技术领域重要的数值与事实型工具书。



从夸克到银河系
海量数据!



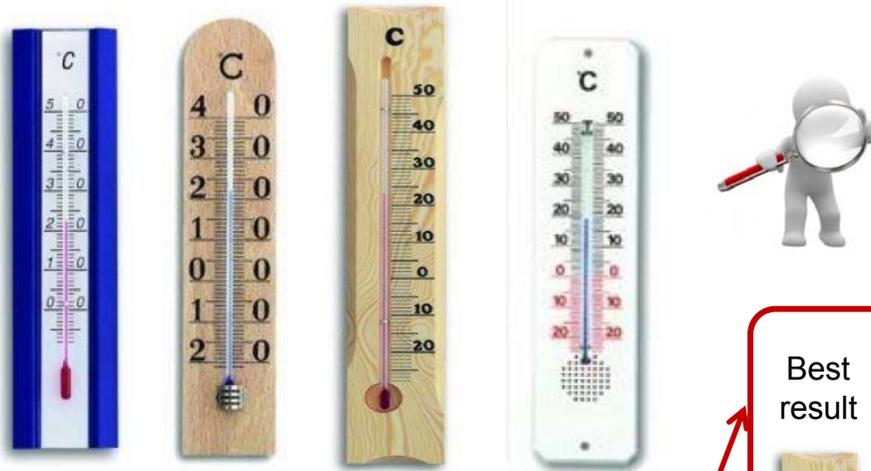
LB工具书的数据

- ✓数据来源于全世界千余名物理与工程领域的科学家撰写的研究期刊全文
- ✓内容涉及相关科学与技术的数值数据（原始数据、图表、试验数据）
- ✓函数关系、常用单位以及基本常数等，还有相关论文与评论等文献
- ✓所有数据都经过严格苛刻的评估和筛选



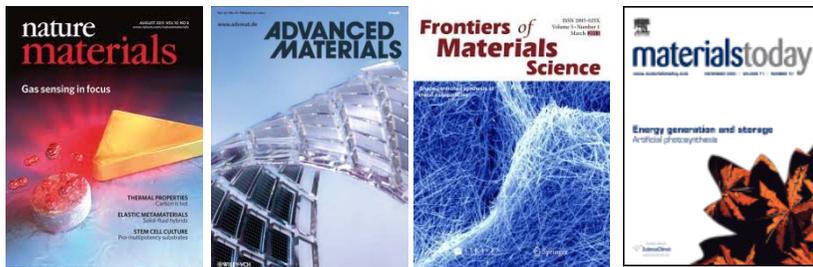
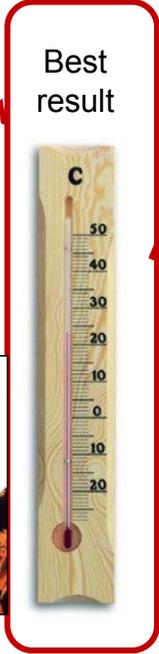
“严格的评估与筛选”意味着什么？

温度



• 数据来自全球各领域的一千多名专家负责对8,000多种经同行评审的期刊原文进行严格苛刻的审阅，评估和筛选，然后将最有效的信息整齐排列和收录。

- 挑选最准确，最可靠的数据
- 描述最佳实验方法和最佳实践操作
- 提供充分背景资料
- 提供原始数据、图表、试验数据、还有相关论文与评论等文献；



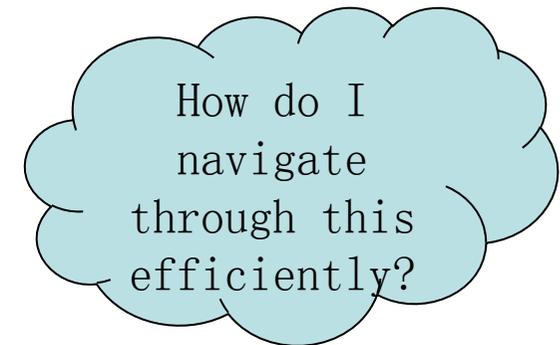
Ref. p. [11]	2. Two-ring system with bridging group	275	
No.	Emp. formula	Thermal temperature [°C]	Ref.
System 3.187 4,4'-disubstituted N-phenyl-2,2,6,6-tetra-tert-butyl-1,3-dioxane-1,3-diol			
1	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
2	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
3	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
System 3.188 4,4'-disubstituted N-phenyl-2,2,6,6-tetra-tert-butyl-1,3-dioxane-1,3-diol			
1	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
2	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
3	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
System 3.189 4,4'-disubstituted N-phenyl-2,2,6,6-tetra-tert-butyl-1,3-dioxane-1,3-diol			
1	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
2	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
3	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
System 3.190 4,4'-disubstituted N-phenyl-2,2,6,6-tetra-tert-butyl-1,3-dioxane-1,3-diol			
1	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
2	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
3	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000

Ref. p. [11]	3. Two-ring system with bridging group	377	
No.	Emp. formula	Thermal temperature [°C]	Ref.
System 3.191 4,4'-disubstituted N-phenyl-2,2,6,6-tetra-tert-butyl-1,3-dioxane-1,3-diol			
1	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
2	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
3	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
System 3.192 4,4'-disubstituted N-phenyl-2,2,6,6-tetra-tert-butyl-1,3-dioxane-1,3-diol			
1	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
2	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
3	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
System 3.193 4,4'-disubstituted N-phenyl-2,2,6,6-tetra-tert-butyl-1,3-dioxane-1,3-diol			
1	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
2	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000
3	C ₂₄ H ₃₆ O ₂	<C ₂₄ H ₃₆ O ₂	C: 0, H: 0, O: 0, A: 0, N: 0, I: 0000



Landolt-Börnstein 工具书分为8部 (group)

- Group I – 基本粒子、原子核和原子
(Elementary Particles, Nuclei and Atoms)
- Group II – 分子和基团(Molecules and Radicals)
- Group III – 聚凝态物质(Condensed Matter)
- Group IV – 物理化学(Physical Chemistry)
- Group V – 地球物理(Geophysics)
- Group VI – 天文学和天体物理学(Astronomy
and Astrophysics)
- Group VII – 生物物理学(Biophysics)
- Group VIII – 先进材料和技术(Advanced Materials
and Technologies)





2001年，Springer 推出 Landolt-Börnstein 在线服务
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 - 半导体
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Springer Materials

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Providing access to numerical and graphical data on the properties of materials

from the Landolt-Börnstein New Series, the Linus Pauling Files and other integrated resources

I

Search by elements

H	He																				
Li	Be															B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar				
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr				
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe				
Cs	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	
Fr	Ra	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Pb	Bi	Po	At	Rn					

Search by structure

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元素检索

结构检索



- graphite

The screenshot shows the Springer Materials search results for the keyword 'graphite'. The interface includes a search bar with 'gra' entered, a list of suggestions, a 'Search by elements' section with a periodic table, and a 'Refine your search' sidebar with three red boxes highlighting 'Data source', 'Discipline', and 'Properties'. The main results area shows 2,532 results for 'Graphite' and lists several articles with titles like 'Some Mechanical Properties of Typical Polymer-Based Composites', 'Introduction', 'Flammability', and '13.2 Raw materials used in the production of hard materials'.

Springer Materials

gra

- Graphite
- Granaticin
- Graniticin
- Gramicidin A
- Gramicidin S
- grain orientation
- grain boundary diffusivity
- Gramicidin S-hydrochlorid-hydrat
- grain size; grain size distribution
- Gramicidin S-dihydrojodidtetrahyd

Search by elements

Refine your search

Data source

- Adsorption 4
- Book Profiles 4
- Inorganic Solid Phases 1738
- Landolt-Börnstein 584
- MSI Eureka 222

Discipline

- Advanced Technologies 801
- Biophysics 950
- Electromagnetism 1314
- Geo- And Astrophysics 43
- Mechanics 210
- Molecules And Radicals 71
- Optics 847
- Particle, Nuclear And Atomic Physics 270
- Solid-State Physics 1198
- Thermodynamics 738

Properties

- A-Value 1
- Absorption 7
- Absorption Coefficient 2
- Absorption Spectrum 1
- Acceptor Energy 1
- Acceptor State 2

2,532 Result(s) for 'Graphite'

Page 1 of 127

Some Mechanical Properties of Typical Polymer-Based Composites

This chapter summarizes some mechanical and physical properties of most used reinforcing agents, thermoplastic and thermosetting resins used as composite matrix, and high performance polymeric matrix composi...

Landolt-Börnstein - Group IV Physical Chemistry

Introduction

This document is part of Subvolume 12A 'Ac-Ag ... Au-Zr, Supplement to Subvolume IV/5A' of Volume 12 'Phase Equilibria, Crystallographic and Thermodynamic Data of Binary Alloys' of Landolt-Börnstein - Group ...

Flammability

The flammability of a polymer is an interaction of pyrolysis, ignition, combustion, flame propagation, and flame extinction processes. The processes are brought about by the heat exposure of the polymer. Hea...

Landolt-Börnstein - Group VIII Advanced Materials and Technologies

13.2 Raw materials used in the production of hard materials

This chapter discusses on the raw materials used in the production of hard materials. Of the many forms of carbon required as the raw material for the conversion to diamond, **graphite** is the most...

Landolt-Börnstein - Group III Condensed Matter

Ac - Mn





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Search by Elements

Search for information by element system

1 H	2 He	3 Li	4 Be	5 B	6 C	7 N	8 O	9 F	10 Ne	11 Na	12 Mg	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe	55 Cs	56 Ba	57 Fr	58 Ra	59 La	60 Ce	61 Pr	62 Nd	63 Pm	64 Sm	65 Eu	66 Gd	67 Tb	68 Dy	69 Ho	70 Er	71 Lu	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn	87 Fr	88 Ra	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr
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Select elements from the periodic table to search by element system.

57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

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Search for information by element system

1 H	2 He																
3 Li	4 Be	5 B	6 C	7 N	8 O	9 F	10 Ne										
11 Na	12 Mg	13 Al	14 Si	15 P	16 S	17 Cl	18 Ar										
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	
87 Fr	88 Ra	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	

Your Selection

Al-Cr-Fe

168 Matching element systems

- Al-Cr-Fe (124)
- Al-Co-Cr-Fe (21)
- Al-Cr-Cu-Fe (1)
- Al-Cr-Fe-Ge (1)
- Al-Cr-Fe-Mn (2)
- Al-Cr-Fe-N (1)
- Al-Cr-Fe-Ni (3)
- Al-Cr-Fe-O (14)
- Al-Cr-Fe-S (1)
- Al-Cr-Fe-Si (1)
- Al-Cr-Cu-Fe-O (2)

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Data Source	
<input type="checkbox"/> Inorganic Solid Phases	62
<input type="checkbox"/> Landolt-Börnstein	18
<input type="checkbox"/> MSI Eureka	44

Discipline	
<input type="checkbox"/> Advanced Technologies	23
<input type="checkbox"/> Biophysics	28
<input type="checkbox"/> Electromagnetism	43
<input type="checkbox"/> Mechanics	1
<input type="checkbox"/> Molecules And Radicals	6
<input type="checkbox"/> Optics	1
<input type="checkbox"/> Particle, Nuclear And Atomic Physics	2
<input type="checkbox"/> Solid-State Physics	46
<input type="checkbox"/> Thermodynamics	82

Properties	
<input type="checkbox"/> Activity	1
<input type="checkbox"/> Antiferromagnetic Neel Temperature	2
<input type="checkbox"/> Arrott Plot	1
<input type="checkbox"/> Atomic Environment	17

124 Result(s) for 'Al-Cr-Fe'

MSI Eureka © 1991 Report ID: 10.14873.1.1

Al-Cr-Fe Ternary Phase Diagram Evaluation

Phase diagrams, crystallographic and thermodynamic data

Thermodynamic calculations of the Al corner of the **Al-Cr-Fe** system by Saunders [...](α Fe)+(γ Fe) surface in the **Al-Cr-Fe** system, based on the microstructural, hardness,...

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Al-Cr-Fe Ternary Phase Diagram Evaluation

Phase diagrams, crystallographic and thermodynamic data

Although the **Al-Cr-Fe** system has undergone many investigations, the **Al-Cr-Fe** equilibrium diagram has not been determined in... ..the (γ Fe)-loop in the **Al-Cr-Fe** system are given...

MSI Eureka © 2007 Report ID: 10.14873.3.4

Al-Cr-Fe Ternary Phase Diagram Evaluation

Phase diagrams, crystallographic and thermodynamic data

...scientific interest in the phase relations in the **Al-Cr-Fe** system, particularly as alloys of this system... ..approximants is also an interesting peculiarity of the **Al-Cr-Fe**

MSI Eureka

Isothermal section at 750°C

Temperature: 750 °C

Concentration Range: Fe conc. [0-100 at.%] vs. Al conc. [0-100 at.%] vs. Cr conc. [0-100 at.%]

Part of report on 'Al-Cr-Fe Ternary Phase Diagram Evaluation'



MSI Eureka

© 1991 Report ID: 10.14873.1.1

Al-Cr-Fe Ternary Phase Diagram Evaluation

Phase diagrams, crystallographic and thermodynamic data

Materials Science International Team, MSIT ©¹ and Gautam Ghosh

Abstract

This report for the ternary system Al-Cr-Fe discusses binary systems, solid phases, invariant equilibria, liquidus surface, and isothermal sections.

Introduction

The major part of the work has been investigated by Kornilov [39Kor, 40Kor1, 40Kor2, 45Kor] and [46Kor] and Kozheurov [70Koz1] and [70Koz2]. Kornilov used Armco grade Fe (0.25 mass% C, 0.05 mass% Si and traces of Mn), Al pigs (0.1 mass% Si, 0.1 mass% Cu), Al powder (0.1 mass% Si, 0.1 mass% Cu), chromium oxide of unspecified purity and analytically pure iron oxide. The alloys were prepared by the aluminothermic process which was also used by other investigators [32Tai1, 32Tai2, 43Mon, 51Pra, 53Cas, 54Chi, 55Tag] and [58Chu]. Thermal analysis was performed to monitor the solidification process, in an induction furnace in insulated corundum crucibles and under an inert atmosphere of He-Ar. [32Tai1] and [32Tai2] used Armco grade Fe (0.14 mass% Si), Al (0.17 mass% Si, 0.6 mass% Fe) and the liquidus surface was determined by thermal analysis. Chubb [58Chu] determined isothermal sections using high-purity Al (99.994 mass%), iodide Cr (99.988 mass%) and electrolytic Fe (99.994 mass%) having extremely low levels of interstitial elements C, H, O, N. Alloys were prepared by arc melting, followed by homogenizing treatment at 1000°C for 100 h. Final heat treatments were done under argon atmosphere in silica capsules and quenched into water. Phase analysis was carried out by optical metallography, X-ray diffraction and hardness testing. [55Tag] and [58Tag] studied the effect of Al addition in Fe-Cr binary alloys on the formation of the σ -phase by means of optical microscopy, X-ray diffraction and hardness measurements.

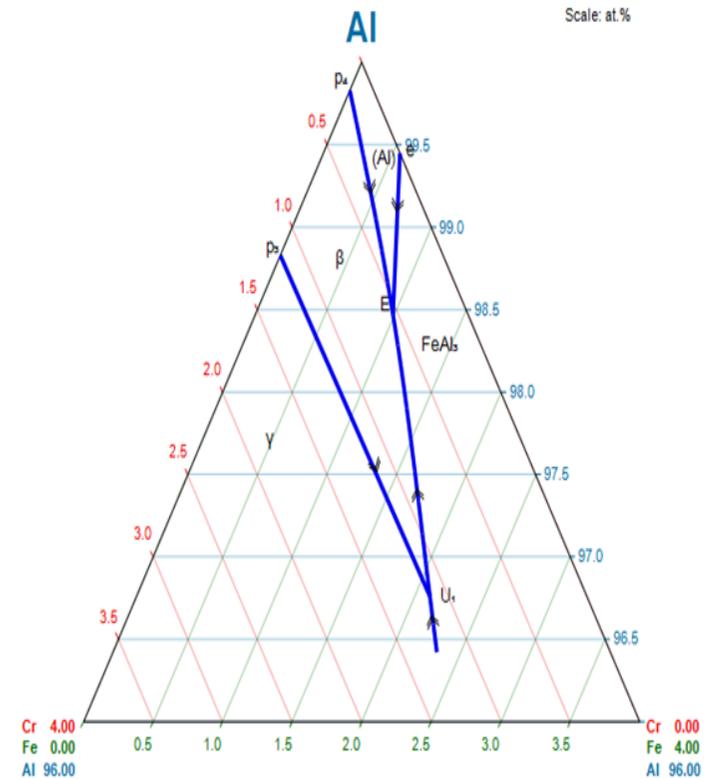


Tables

Table 1
Solid Phases

Phase/ Temperature Range (°C)	Pearson Symbol/ Prototype	Lattice Parameters (pm)	Comments
(Al) ≤880.452	cF4 Cu	a = 404.88	pure Al at 24°C [V-Q]
(Cr,αFe) Cr ≤1883 (αFe)(r) ≤912	 cI2 W	 a = 288.4 a = 286.65	 (Cr) and (αFe) completely soluble, Al solubility both in (Cr) and in (αFe) ≈ 46 at. % [Mas] pure Cr at 27°C [V-Q] pure Fe at 20°C [V-Q]

Fig. 2: Liquidus projection of the Al-corner



MSI Fig. 2: Liquidus projection of the Al-corner



- benzene

Search by Structure

Start by drawing a structure



1578 Result(s) for this structure

Page 1 of 79

Benzene

Molecular Formula: C_6H_6

Inchi: InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H

Molecular Mass: -

Inchi Key: UHOVQNZJYSORNB-

CAS-No:

UHFFFAOYSA-N

174973-86-1,54682-86-9,71-43-2

[» View substance profile](#) [» Search for this substance](#)



100 % match

C_7H_6

Molecular Formula: C_7H_6

Inchi: InChI=1S/C7H6/c1-2-4-7-5-6(7)3-1

Molecular Mass: -

/h1-4H,5H2

CAS-No: 4646-69-9

Inchi Key: AMSMVCOBZOZLEE-UHFFFAOYSA-N

[» View substance profile](#) [» Search for this substance](#)



86 % match

Toluene

Molecular Formula: C_7H_8

Inchi: InChI=1S/C7H8/c1-7-5-3-2-4-6-7/h2-6H,1H3

Molecular Mass: -

Inchi Key: YXFVWABEGXRONW-UHFFFAOYSA-N

CAS-No: 108-88-3

[» View substance profile](#) [» Search for this substance](#)



84 % match

Benzenamine

Molecular Formula: C_6H_7N

Inchi: InChI=1S/C6H7N/c7-6-4-2-1-3-5-6

Molecular Mass: -

/h1-5H,7H2

CAS-No:

Inchi Key: PAYRUJLWNCNPSJ-UHFFFAOYSA-N

146997-94-6,37342-16-8,62-53-3

[» View substance profile](#) [» Search for this substance](#)



83 % match



检索结果分类:

- 3D Interactive Structure
- Information on SMs
- Chemical Properties+Synthesis

Benzene

General information

Molecular Formula: C_6H_6
Element System: C-H
CAS-RN: 174973-66-1, 54682-86-9, 71-43-2
InChI: InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H



[View 3D Interactive Structure](#)

3D Interactive Structure

Information on SpringerMaterials

Properties frequently appearing with benzene

» Osmotic Pressure (479)	» Phase Equilibrium (211)	» Solid Liquid Equilibrium (75)
» Heat Of Mixing (376)	» Density (127)	» Refractive Index (65)
» Excess Enthalpy (376)	» Excess Volume (89)	» Activity (62)
» Heat Of Solution (330)	» Dielectric Constant (77)	» Viscosity (53)
» Vapor-Liquid Equilibrium (276)	» Permittivity (76)	» Mixing Enthalpy (46)
» See More		

Chemical Properties + Synthesis

Molecular Weight: 78.1134
Calculated Log P: 1.906
Rotatable Bonds: 0
H Acceptors: 0
H Donators: 0
Reactions having this substance as a reactant: 29676
Reactions having this substance as a product: 1192

Journal articles containing this substance: 4017
Patents containing this substance: 1382
Other publications containing this substance: 551
Suppliers: ABCR, Alfa Aesar, Apollo Scientific, Otava, Sigma-Aldrich, VWR



学科馆员

中国科学院国家科学图书馆

- 3D Interactive Structure

Benzene

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InChI: InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H

[View 3D Interactive Structure](#)

3D Interactive Structure

More Options ▾

Modify display:

- Bonds Between Atoms
- Atoms
- Polyhedra
- Spin

Measurement options:

- Distance Measurement
- Angle Measurement
- Torsion Angle Measurement
- Deactivate measurement options

Export Options ▾

- Export JPG Image
- Export PNG Image

Export Options ▾

More Options ▾



● Information on SMs——Band gap

Benzene

General information

Molecular Formula: C_6H_6
Element System: C-H
CAS-RN: 174973-66-1, 54682-86-9, 71-43-2
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[View 3D Interactive Structure](#)

3D Interactive Structure

Information on SpringerMaterials

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- » Heat Of Mixing (376)
- » Excess Enthalpy (376)
- » Heat Of Solution (330)
- » Vapor-Liquid Equilibrium (276)
- » See More
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Information on SpringerMaterials

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- » Solid Liquid Equilibrium (75)
- » Refractive Index (65)
- » Activity (62)
- » Viscosity (53)
- » Mixing Enthalpy (46)
- » Diffusion (39)
- » Chemical Diffusion (38)
- » Sound Velocity (36)
- » Heat Capacity (32)
- » Surface Tension (31)
- » Solid-Liquid Phase Equilibrium (28)
- » Composition (16)
- » Chemical Composition (16)
- » Adsorption (15)
- » Virial Coefficient (14)
- » Polarization Degree (13)
- » Luminescence Emission Linewidth (13)
- » Luminescence (13)
- » Heat Conductivity (12)
- » Thermal Conductivity (12)
- » Dilution Enthalpy (10)
- » Crystal Structure (7)
- » Band Structure (7)
- » Isentropic Compressibility (6)
- » Compressibility (5)
- » Effective Mass (4)
- » Unit Cell Parameter (4)
- » Melting Temperature (4)
- » Hole g-Factor (4)
- » Band Gap (4)
- » Mobility (4)
- » Dielectricity (3)
- » Electronic Structure (3)
- » Photoemission Spectroscopy (3)
- » Internuclear Distance (3)
- » Phase Transition (3)
- » Photoemission (3)
- » Quadrupole Coupling (3)
- » Core Level Transition (3)
- » Valence Band (3)
- » Critical Point (3)
- » Nuclear Quadrupole Coupling (2)
- » Space Group (2)
- » Acentric Factor (2)
- » Transition Enthalpy (2)
- » Differential Scanning Calorimetry (2)
- » Rotational Excitation Cross Section (2)
- » Heat Of Fusion (2)
- » Boiling Point (2)
- » Magnetic Susceptibility (2)
- » Centrifugal Distortion (2)
- » Rotation-Vibration Spectrum (2)
- » Liquid-Liquid Equilibrium (2)
- » Molar Heat Capacity (2)
- » Diamagnetic Susceptibility (2)
- » Formula Unit (2)
- » Vapor Pressure (2)
- » Dipole Moment (2)
- » Point Group (2)
- » Unit Cell (2)
- » Phonon Wavenumber (1)
- » Expansion Coefficient (1)
- » Coupling Constant (1)
- » Piezoelectric Effect (1)
- » Enthalpy (1)
- » Exaltation Data (1)
- » ^{13}C Nuclear Magnetic Resonance Spectrum (1)
- » Phase Diagram (1)
- » Magnetic Susceptibility Exaltation (1)
- » Angular Frequency (1)
- » Absorbance (1)
- » Exciton Fine Structure (1)
- » Grain Size (1)
- » Phase Transition Temperature (1)
- » Magnetic Anisotropy (1)
- » Gibbs Energy (1)
- » Piezoelectric Constant (1)
- » Molar Mass (1)
- » Self-Diffusion (1)
- » Equilibrium Structure (1)
- » Diffusion Of Impurities (1)
- » Absorption (1)
- » Charge Carrier Mobility (1)
- » Impurity Concentration (1)
- » Formation Entropy (1)
- » Elastic Coefficients (1)
- » Diamagnetic Susceptibility Exaltation (1)
- » Migration Energy (1)
- » Chemical Shift (1)
- » Dispersion (1)
- » Transition Entropy (1)
- » Structure Data (1)
- » Formation Enthalpy (1)
- » Reaction Coordinate (1)
- » Radical Ion State (1)
- » Potential Energy (1)
- » Creep (1)
- » Formation Energy (1)
- » Dunham Energy Parameter (1)
- » Nuclear Quadrupole Resonance Spectroscopy (1)
- » Latent Heat (1)
- » Heat Of Sublimation (1)
- » Heat Of Transition (1)
- » Entropy (1)
- » Coriolis Coupling (1)
- » Tracer Diffusion (1)
- » Shock Waves (1)
- » Asymmetry Parameter (1)
- » Nuclear Magnetic Resonance (1)
- » Melting Curve (1)



Information on SMs

Springer Materials

Benzene

Home • Contact us

Refine your search

Data source
 Landolt-Börnstein 4

Discipline
 Biophysics 2
 Electromagnetism 4
 Mechanics 1
 Optics 4
 Solid-State Physics 4
 Thermodynamics 1

Properties
 Band Gap 4
 ¹³C Nuclear Magnetic Resonance Spectrum 1
 Absorbance 1
 Absorption 1
 Acentric Factor 2
 Activity 62
 Adsorption 15
 Angular Frequency 1

4 Result(s)
Substance: Benzene Properties: Band Gap

Landolt-Börnstein - Group III Condensed Matter
Benzene, C₆H₆ elastic moduli, n
This document is part of Subvolume E 'Ternary Compounds, Organic Semiconductors' of Volume 41 'Semiconductors' of Landolt-Börnstein - Group III Condensed Matter.

Landolt-Börnstein - Group III Condensed Matter
Benzene, C₆H₆ exciton paramet
This document is part of Subvolume E 'Ternary Compounds, Organic Semiconductors' of Volume 41 'Semiconductors' of Landolt-Börnstein - Group III Condensed Matter.

Landolt-Börnstein - Group III Condensed Matter
Benzene, C₆H₆ charge carrier m
This document is part of Subvolume E 'Ternary Compounds, Organic Semiconductors' of Volume 41 'Semiconductors' of Landolt-Börnstein - Group III Condensed Matter.

Landolt-Börnstein - Group III Condensed Matter
Benzene, C₆H₆ crystal structure
This document is part of Subvolume E 'Ternary Compounds, Organic Semiconductors' of Volume 41 'Semiconductors' of Landolt-Börnstein - Group III Condensed Matter.

Landolt-Börnstein - Group III Condensed Matter

Benzene, C₆H₆ crystal structure, lattice parameters

Abstract

This document is part of Subvolume E 'Ternary Compounds, Organic Semiconductors' of Volume 41 'Semiconductors' of Landolt-Börnstein - Group III Condensed Matter.

Download Chapter

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1 / 3

自动缩放

substance: benzene, C₆H₆
property: crystal structure, lattice parameters

For symbols, definitions and abbreviations, see [] for general remarks on organic semiconductors, see [] on wide gap photoconductive semiconductors also []

molecular structure

crystal structure
orthorhombic, space group D_{2h}¹⁵ - Pbc_a, Z = 4

lattice parameters

<i>a</i>	7.460	<i>T</i> = 270 K	X-ray diffraction	58C
<i>b</i>	9.666			
<i>c</i>	7.034			
<i>a</i>	7.38	<i>T</i> = 103 K	X-ray diffraction	55K
<i>b</i>	9.57			
<i>c</i>	6.74			
<i>a</i>	7.292	<i>T</i> = 78 K	X-ray diffraction	55K
<i>b</i>	9.471			
<i>c</i>	6.742			

molecular packing diagram: see Fig. 1



适用的行业

- Chemicals 化工产品
- IT & Semiconductors 计算机&半导体
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- Photovoltaics 光伏材料
- Glass & Ceramics 玻璃和制陶业
- Metals & Mining 冶金和矿产
- Engineering 工程
- Petrochemistry 石油化工
- Automotive 汽车业
- Electronics 电子工业
- Aerospace & Defence 航空与国防
- Energy 能源
- Oil & Gas 石油

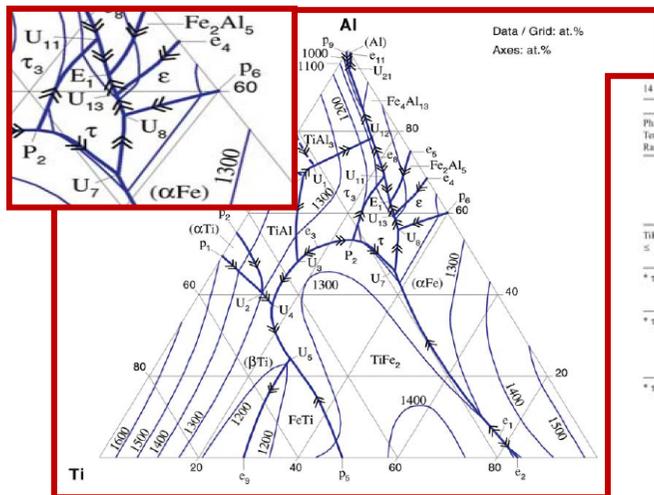




利用Springer Materials准备课题 或者对试验结果进行分析

例如：利用Springer Materials查找材料参数

- 利用专业知识库进行可靠的新材料设计
- 为研究项目找出哪种材料能够提供最可靠的匹配参数
- 在实际测量完毕以后与已知的材料参数进行对比、评估与证实试验所获得的数据



Phase/ Temperature Range [°C]	Pearson Symbol/ Space Group/ Prototype	Lattice Parameters [pm]	Comments/References
		$a = 496.61$ $c = 806.28$	[2006Van], $\text{Ti}_{13}\text{Fe}_{13}\text{Al}_{13.4}$ annealed at 1000°C
		$a = 503.66$ $c = 819.71$	[2000Van], as-cast $\text{Ti}_{13}\text{Fe}_{13}\text{Al}_{13}$
TiFe ≤ 1317	$cP2$ $Fm\bar{3}m$ GdCl ₃	$a = 297.6$	solid solubility ranges from 49.8 to 51.8 at.% Ti [V-C]
* τ_1 , TiFe ₂ Al	$cP14$ $Fm\bar{3}m$ $C_{2v}AMn$	$a = 587.9$	[1983Hsu], annealed at 900°C for 14 days
* τ_2	cP^* $F43m$	$a = 1211.0$ $a = 1209.59$	[1995Phi], at $\text{Ti}_{10}\text{Fe}_{12}\text{Al}_{12.6}$ [2006Gry], $\text{Ti}_{10}\text{Fe}_{12}\text{Al}_{12}$ annealed at 900°C, both X-ray and neutron diffraction data
* τ_2'	$cP116$ $Fm\bar{3}m$ $\text{Th}_3\text{Mn}_{12}$	$a = 1199.0$ $a = 1182.0$ $a = 1203.8$ $a = 1207.6$ $a = 1209.9$ $a = 1211.0$ $a = 1189.0$	[1967Mac, 2000Mah] [1981Sci] [1995Phi], at $\text{Ti}_{10.8}\text{Fe}_{12.1}\text{Al}_{12.4}$ [1999Gor], at $\text{Ti}_{10.4}\text{Fe}_{12.1}\text{Al}_{12.5}$ [1999Gor], at $\text{Ti}_{10.2}\text{Fe}_{12.1}\text{Al}_{12.7}$ [1999Lev] [2003Gry], at $\text{Ti}_{10.8}\text{Fe}_{12.1}\text{Al}_{12.6}$
filled $\text{Th}_3\text{Mn}_{12}$		$a = 1209.2$	[2003Gry], at $\text{Ti}_{10}\text{Fe}_{12.1}\text{Al}_{12.7}$
filled $\text{Th}_3\text{Mn}_{12}$		$a = 1199.44$	[2006Gry], $\text{Ti}_{10}\text{Fe}_{12}\text{Al}_{12}$ annealed at 900°C, neutron diffraction data



飞机设计师需要寻找制作高强度机翼的新型铝合金材料，例如：Al-Fe-Ti



SpringerMaterials包含的材料种类

Metals
金属

Ceramics
陶瓷

Nuclear physics
原子物理

Semiconductors
半导体

Thin Films

Nano Powders
纳米粉

Biomaterials
生物材料

Nanotubes
纳米管

Organic Materials
有机材料

Composite Materials
复合材料

Nanomaterials
纳米材料



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中国科学院国家科学图书馆

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大型的 全面的 重要的 系统的 权威的 可信的

使用： 方便的 快捷的

全院开通 免费





● Reaxys组成

Beilstein

有机化学

(始于1771)

- ☞ 全球最全的有机化学数值和事实库
- ☞ 化学结构相关的化学、物理等方面的性质；化学反应相关的各种数据
- ☞ 详细的药理学，环境病毒学，生态学等信息资源

Gmelin

无机化学

(始于1772)

- ☞ 当今最全面的无机与金属有机化学数值与事实数据库
- ☞ 详细的理化性质，地质学，矿物学，冶金学，材料学等方面的信息资源

PCD

化学专利

(始于1976)

- ☞ 化学专利数据库
- ☞ 世界知识产权组织，美国专利局，欧洲专利局专利信息



☺ Reaxys数据

A Bibliographic Database

>46 million records
(from ~16,000 journal titles plus records from key patent organisations)

A Substance Database

> 78 million substances (total)
~ 57 million substances (unique)

Reaxys

A Chemical Reaction Database

> 36 million reactions

A Property Database

> 500 million experimental properties
in > 500 fields
in > 130 subject areas

INTEGRATED DATABASES

PubChem

BioAssay Compound Substance

eMolecules

Linking researchers needs to supplier capabilities

INTEROPERABILITY WITH

Scopus

ScienceDirect



- **~57.0 Million unique Substances**
- **~36.6 Million Reactions**
- **~500 Million experimental properties**
- **~16,000 Journal Titles**
(Life Science, Chemistry&Engineering,
Pharmacology, Enviromental Science, Books, Conference
proceedings, Editorials etc.)
- **~46 Million Bibliographic Records**
- **> 500 Search fields(through querylet)**

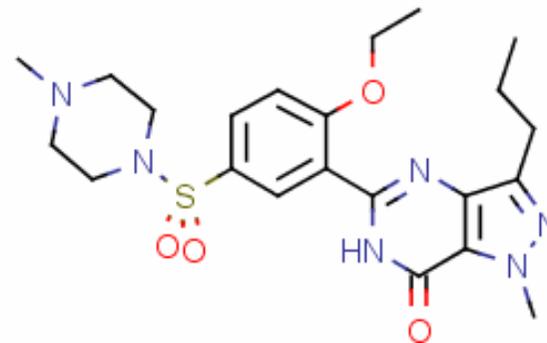




解决的问题

1. 是什么?

- 新物质? 专利保护?
- 物化性质(密度, 粘度, 折射率, 生成焓等)?



2. 什么用途?

- 反应物? 溶剂? 催化剂?
- 生物活性? 药理性质?
- 毒性?

Fabrication of Ordered ZnO/TiO₂ Heterostructures via a Templating Technique

Jian F. Lei [✉], Li B. Li [†], Xue H. Shen [‡], Kai Du [†],
Jing Ni [†], Chao J. Liu [†], and Wei S. Li [§]
[†] School of Physics and Engineering, Henan University
of Science and Technology, Luoyang 471023, China
[‡] College of Life Science, Tarim University, Alar
843300, China
[§] School of Chemistry and Environment, South China
Normal University, Guangzhou 510006, China

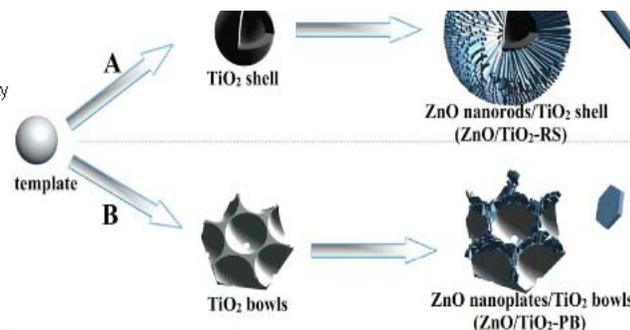
Langmuir, Article ASAP

DOI: 10.1021/la4027859

Publication Date (Web): October 16, 2013

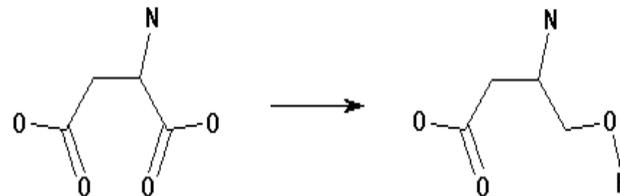
Copyright © 2013 American Chemical Society

[✉]E-mail: leijianfei9966@163.com. Telephone and fax: 86-375



3. 怎样得到?

- 已知制备方法?
- 对制备方法进行改进?





Reaxys专门服务于从事有机化学、无机化学、
有机金属化学及相关学科的

- ◆ 药物化学家
- ◆ 合成化学家
- ◆ 过程工程师
- ◆ 化工工程师
- ◆ 材料化学家



REAXYS: SIMPLER TO SEARCH, MORE DISCOVERABLE INFORMATION

The screenshot shows the Reaxys website interface with several Chinese annotations in blue boxes:

- 快速智能检索** (Fast intelligent search) is placed over the search bar.
- 化合物** (Compounds) is placed over the 'Substances' icon.
- ReaxysTree** is placed over the 'ReaxysTree' icon.
- 谱图** (Spectra) is placed over the 'Spectra' icon.
- 高级检索** (Advanced search) is placed over the 'Advanced' icon.
- 反应** (Reactions) is placed over the 'Reactions' icon.
- 文献** (Literature) is placed over the 'Literature' icon.
- 物理性质** (Physical properties) is placed over the 'Physical' icon.
- 天然产物** (Natural products) is placed over the 'Natural Product' icon.

The interface includes a navigation menu (Query, Results, Synthesis Plans, History, Report, My Alerts, My Settings, Help, Register), a search bar with a 'Go' button, and a grid of search categories. Below the grid, there is a section for 'ReaxysTree' with a search bar and a list of sub-categories: chemical transformations, physico chemical analysis methods, physico chemical properties, and quantum chemical calculation methods. A 'Search Literature' button is located at the bottom right.



快速智能检索

- “publications about polylactic acid”
- “preparation of polylactic acid”

The screenshot displays a chemical database search interface with the following components:

- Navigation:** Tabs for Reactions (909), Substances (1307), and Citations (12142). A search bar and navigation controls are at the top right.
- Search Results Table:**

Item	Title of the Document	Authors
1	Natureworks PLA: Sustainable performance fiber	Dartee; Lunt; Sha
2	Preparation and testing of polylactic acid ultra thin fiber membrane as the sustained release material	Jianxiang, Yu; Tai
3	Application of polylactic acid in hot melting sizing for worsted yarns	Liu, Yu; Wang, Sh
- Reaction Details:**
 - Reaction 1:** No structure RN: 8187546. Product: CC(O)C(=O)O. Rx-ID: 38195196. Conditions: With ErCl_3 in water, T=240°C; P=15001.5 Torr; 0.5 h; Inert atmosphere. Yield: 83.2%.
 - Reaction 2:** CC(N)C(=O)O → CC(O)C(=O)O. Rx-ID: 197864. Conditions: With sulfuric acid; sodium nitrite in water, T=0°C; 12 h. Yield: 65%.
- References:** Applied Catalysis A: General, 2014, vol. 482, p. 78 - 83. Authors: Lei, Xing; Wang, Fen-Fen; Liu, Chun-Ling; Yang, Rong-Zhen; Dong, Wen-Sheng.



反应检索

Structure

selected query editor:
 MarvinSketch
by ChemAxon

PASTE STRUCTURE EDITOR

Create Structure Template from Name

As drawn
 Substructure
 on heteroatoms
 on all atoms
 Similarity

Include tautomers
 Ignore stereo
 No isotopes
 No charges
 No radicals
 No ring closures
 Ignore atom mappings
 Align results with query
 Keep fragments
 separate together

化学结构其他检索条件限定

结构限定

Please select role Product Starting material Reagent / Catalyst Any role

反应角色限定

Reaction Data

Yield (numerical)	=	<input type="text"/>	Lookup X
Solvent	is	<input type="text"/>	Lookup X
Reagent/Catalyst	is	<input type="text"/>	Lookup X
Time (h)	=	<input type="text"/>	Lookup X
Temperature (°C)	=	<input type="text"/>	Lookup X
Pressure (Torr)	=	<input type="text"/>	Lookup X
Reaction Type	is	<input type="text"/>	Lookup X

反应数据限定

Search Reactions



物质检索



Reactions



Substances



Literature



ReaxysTree



Physical



Spectra



Natural Product



Advanced

Structure



selected query editor:



MarvinSketch
by ChemAxon

PASTE

STRUCTURE EDITOR

- As drawn
- Substructure
 - on heteroatoms
 - on all atoms
- Similarity

- Include tautomers
- Ignore stereo
- No salts
- No mixtures
- No isotopes
- No charges
- No radicals
- No ring closures
- Align results with query

More options

Create Structure Template from Name

Identification

Reaxys Registry Number	=	<input type="text"/>	Lookup	×
CAS Registry Number	is	<input type="text"/>	Lookup	×
Chemical Name	is	<input type="text"/>	Lookup	×
Element Symbols	is	<input type="text"/>	Lookup	×

Show AND Buttons

Search Substances



Ask Reaxys



Enter a keyword, concept or author

Go



Reactions



Substances



Literature



ReaxysTree



Physical



Spectra



Natural Product



Advanced

Bibliographic Data

Document Type

is

Lookup X

Authors

is

Lookup X

Common Patent Number

is

Lookup X

Patent Country Code

is

Lookup X

Journal Title

is

Lookup X

Publication Year

=

Lookup X

DOI

is

Lookup X

Title

is

Lookup X

Abstract

is

Lookup X

Keywords

is

Lookup X

Citation Basic Index

is

Lookup X

Show AND Buttons

Search Literature

Add to Query:

Structure

Molecular Formula

Alloy

Add/Remove Fields...



ReaxysTree检索

按Reaxys数据库的系统分类，进行选择、检索

The screenshot displays the ReaxysTree web interface. At the top, a navigation bar includes links for Query, Results, Synthesis Plans, History, Report, My Alerts, My Settings, and Help. Below this is a search bar labeled "Ask Reaxys" with a "BETA" badge and a "Go" button. A row of icons represents different database categories: Reactions, Substances, Literature, ReaxysTree (highlighted with a red border), Physical, Spectra, Natural Product, and Advanced. The "Browse Literature" section is active, showing a search input field and a list of categories. The "ReaxysTree" category is selected, and a red box highlights the "quantum chemical calculation methods" category in the left sidebar. An arrow points from this box to a detailed view of this category on the right, which lists sub-categories such as "ab initio calculation", "coupled cluster theory", "electron correlation and CI calculation", "relativistic calculation", and "valence bond calculation".

Query Results Synthesis Plans History Report My Alerts My Settings Help

← Start Over

Ask Reaxys **BETA** Enter a keyword, concept or author Go

Reactions Substances Literature **ReaxysTree** Physical Spectra Natural Product Advanced

Browse Literature
Look through the Reaxys data by browsing its hierarchy of entities and properties. Select items and click Search

Find any term SEARCH

Reset Select All Highlighted Deselect All

- ReaxysTree
 - chemical transformations (chemical reaction classification, chemical reaction classifications, chemical transformation...)
 - physico chemical analysis methods (chemical analysis, chemical analysis method, determination method, physico chemical a...)
 - physico chemical properties (physico chemical magnitude, physico chemical magnitudes, physico chemical property,...)
 - quantum chemical calculation methods** (quantum chemical calculation method, Quantum chemical calculations)

- quantum chemical calculation methods (quantum chemical calculation method, Quantum chemical calculations)
 - ab initio calculation (ab initio calculations, ab initio MO calculation, ab initio molecular orbital calculation, Hart...)
 - coupled cluster theory (CC model, CC theory, coupled cluster calculation, coupled cluster model)
 - coupled cluster singles and doubles theory (CCSD calculation, CCSD theory, coupled cluster singles and doubles)
 - electron correlation and CI calculation (Electron correlation and CI calcn., electron correlation and CI calculations)
 - electronic band structure model (electronic band structure calculation, theory of band structure, theory of band structur...)
 - empirical method (Empirical methods)
 - relativistic calculation (relativistic calculations, relativistic quantum chemistry)
 - semi-empirical NDO calculation (PCILO) MINDO INDO Semi-empirical NDO calcns. (CNDO, semi-empirical NDO calculati...)
 - statistical model calculation (statistical model calculations)
 - valence bond calculation (valence bond calculations, valence bond theory, VB model, VB theory)



物理检索

Ask Reaxys



Enter a keyword, concept or aut

宏观数据: 熔点, 沸点, 临界参数, 饱和蒸
汽压, 折射率, 热容, 摩尔蒸发焓等。
微观数据: 分子偶极矩, 电离能, 键参数
(键角、键长、键能) 等。

Reactions Substances Literature ReaxysTree **Physical**

Physical Data

Melting Point (°C)	=		Lookup	×
Boiling Point (°C)	=		Lookup	×
Refractive Index	=		Lookup	×
Density	<input type="checkbox"/>	exists		×
Dissociation Exponent	<input type="checkbox"/>	exists		×
Dynamic Viscosity (P)	=		Lookup	×
Optical Rotatory Power (deg)	=		Lookup	×
log POW	=		Lookup	×

Show AND Buttons

Add to Query:

Structure

Molecular Formula

Alloy

Add/Remove Fields...

Search Substances



Ask Reaxys



Enter a keyword, concept or author

Go



Reactions



Substances



Literature



ReaxysTree



Physical



Spectra



Natural Product



Advanced

Spectra

NMR Spectroscopy

exists

×

Nucleus

is

Lookup

×

IR Spectroscopy

exists

×

Description

is

Lookup

×

Mass Spectrometry

exists

×

Description

is

Lookup

×

UV/VIS Spectroscopy

exists

×

Description

is

Lookup

×

ESR Spectroscopy

exists

×

Description

is

Lookup

×

Show AND Buttons

Add to Query:

Structure

Molecular Formula

Alloy

Add/Remove Fields...

Search Substances



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天然产物检索



Xiang Shen (shenx@mail.las.ac.cn) is logged in

Query Results Synthesis Plans History Report My Alerts My Settings Help

Logout

Start Over

Import Save

Ask Reaxys



Enter a keyword, concept or author

Go



Reactions



Substances



Literature



ReaxysTree



Physical



Spectra



Natural Product



Advanced

Natural Product

Isolation from Natural Product

exists

×

Isolation from Natural Product

is

Lookup ×

Show AND Buttons

Add to Query:

Structure

Molecular Formula

Alloy

Add/Remove Fields...

Search Substances

Clear Query



Structure

selected query editor:

MarvinSketch
by ChemAxon

As drawn Include tautomers
 Substructure Ignore stereo
 on heteroatoms No salts
 on all atoms No mixtures

Advanced

Construct a query by typing or use the field list.

`IDE.CN='$, $-diphenylalanine hydrochloride' AND IDE.FMF='AcH8O4'` [Check Syntax](#)

[Hide Property List](#)

Find any property with a few characters... e.g., bond type

Available Properties

- Reaxys
 - Identification exists
 - Substance Identification
 - Reaxys Registry Number (IDE.XRN)
 - Preferred RN (IDE.XPR)
 - CAS Registry Number (IDE.RN)
 - Chemical Name (IDE.CN)
 - Chemical Name Segment (IDE.CNS)
 - Linear Structure Formula (IDE.LSF)

Specify complex property queries in this format: "<field code> <operator> <field value(s)>". Click any property in the outline to add its code to your query. [More Syntax Details](#)

选择, Transfer

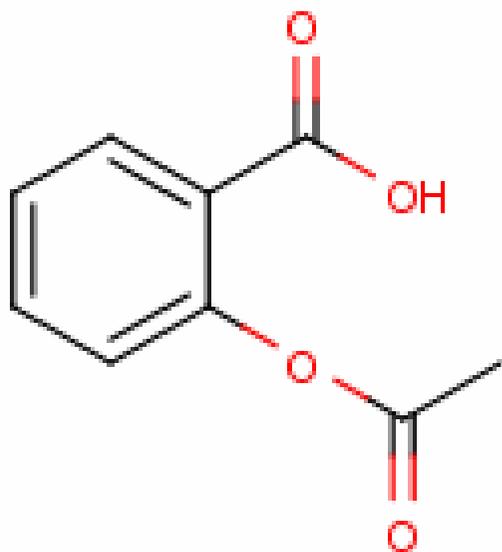
Create Structure Template from

Please select role Product

Advanced

Construct a query by typing

Example: IDE.MW=?
molecular weight
elements (NE) is



检索反应
设计合成路线



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Structure

selected query editor:
 **MarvinSketch**
by ChemAxon

点击、启动
Java、打开
结构编辑器

As drawn
 Substructure
 on heteroatoms
 on all atoms
 Similarity

Please select role Product Starting material Reagent / Catalyst Any r

Reaction Data

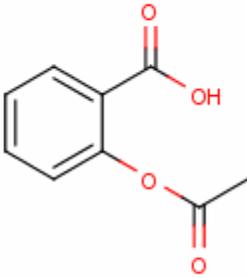
Yield (numerical)	=	
Solvent	is	
Reagent/Catalyst	is	
Time (h)	=	
Temperature (°C)	=	
Pressure (Torr)	=	
Reaction Type	is	

File Edit View Insert Options Object Templates Chemistry Calculations Help

绘制结构

Marvin Sketch

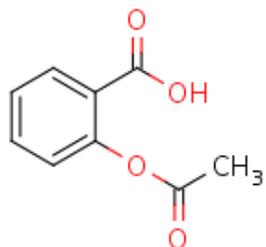
还支持
CrossFire SE;
Symyx Draw;
Symyx ISIS Draw;
CambridgeSoft
ChemDraw



Transfer Query

Cancel & Return

Reaxys supports various structure editors. Please check "My Settings" for more.



- As drawn
- Substructure
 - on heteroatoms
 - on all atoms
- Similarity

PASTE

EDIT

CLEAR

Create Structure Template from Name

Please select role Product Starting material Reagent / Catalyst

Reaction Data

Yield (numerical)

Solvent

Reagent/Catalyst

Time (h)

Temperature (°C)

Pressure (Torr)

Reaction Type

Reaction Basic Index

Show AND Buttons

=

<

<<

>

>>

=

=

=

=

=

is

is

starts with

ends with

contains

ethan|
ethanol
ethane
ethane 1,2-dithiol
ethane-1,2-diamine
ethane-1,2-diol
ethane-1,2-dithiol
ethanedioic acid dihydrate
ethanediol methyl ether
ethanedithiol; 1,2-
ethanesulfonic acid
ethanethioamide
ethanethiol
ethanethiolic acid

Lookup X

Select index items and click 'Transfer'

Reaxys

Search for: ethan

ethanol (1)
ethane (5)
ethane 1,2-dithiol (2)
ethane-1,2-diamine (5)
ethane-1,2-diol (52)
ethane-1,2-dithiol (9)
ethanedioic acid dihydrate (1)
ethanediol methyl ether (2)
ethanedithiol; 1,2- (1)
ethanesulfonic acid (1)
ethanethioamide (3)
ethanethiol (1623)
ethanethiolic acid (20)
ethanol (2)
ethanol (1)
ethanol (2)
ethanol (4)
ethanol (4)
ethanol; (1)
ethanol (4111556)

可多选

Transfer

Reset

Cancel

Page 312 of 572

Add to Query:

Structure

Molecule

Alloy

Add/Remove Fields...

Search Reactions

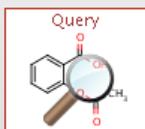


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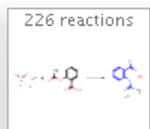
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Query Results Synthesis Plans History Report My Alerts My Settings Help

Logout



Create Alert



筛选限定

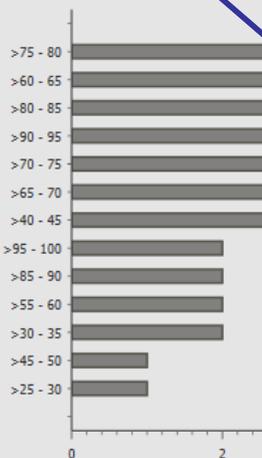
Filter by:

- Sub-structure
- Yield
- Record Type
- Reagent/Catalyst
- Solvent
- Reaction Type
- No. of Steps
- Product Availability
- Reactant Availability
- Availability in other DBs
- Molecular Weight
- Number of Fragments
- Physical Data

Open Analysis View

226 reactions out of 334 substances and 208 citations

Histogram A Yield



- Catalysts (classified)
- Reactions (classified)
- Reagent/Catalyst
- Solvent
- Solvents (classified)
- Yield

- Compounds (classified)
- Boiling Point
- Density
- Melting Point
- Molecular Formula
- Molecular Weight
- Pharmacological Effects
- Physical Data
- Solubility
- Spectroscopic Data

- Document Type
- Authors
- Patent Assignee
- Journal Title
- Publication Year

Close Analysis View

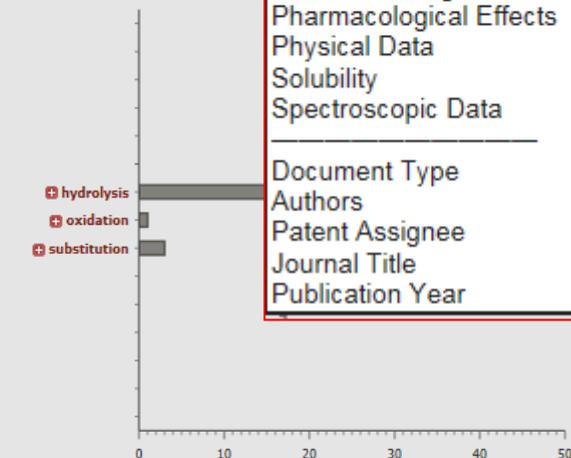
Use your mouse to select or de-select bins for filtering

226 reactions out of 334 substances and 208 citations

Limit to Exclude

Histogram B Reactions (classified)

Reactions (classified)

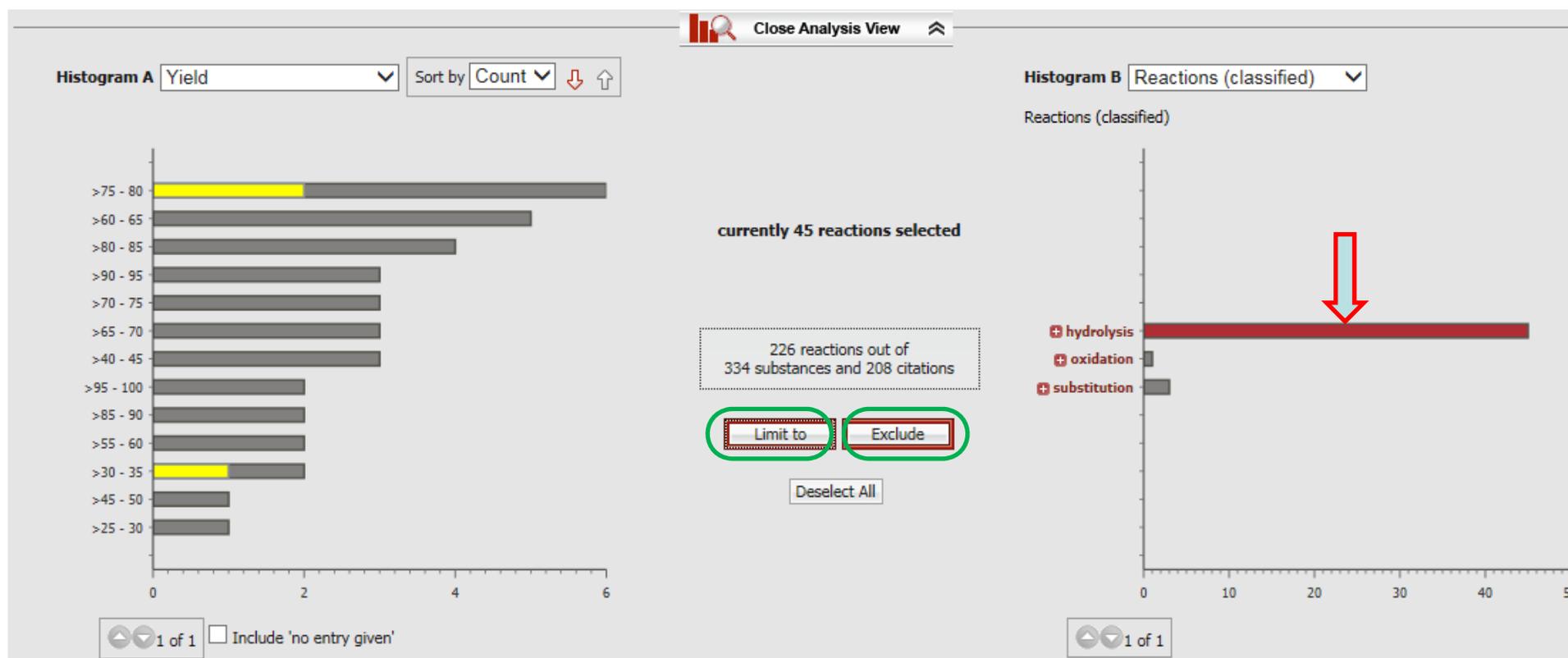


- Catalysts (classified)
- Reactions (classified)
- Reagent/Catalyst
- Solvent
- Solvents (classified)
- Yield

- Compounds (classified)
- Boiling Point
- Density
- Melting Point
- Molecular Formula
- Molecular Weight
- Pharmacological Effects
- Physical Data
- Solubility
- Spectroscopic Data

- Document Type
- Authors
- Patent Assignee
- Journal Title
- Publication Year

1 of 1





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Query

Results

Synthesis Plans

History

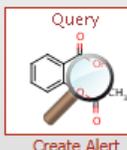
Report

My Alerts

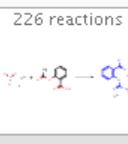
My Settings

Help

Logout



Create Alert



图形导航器：双击即可定位其中任一检索环节

创建Alerts

Filter by:

Sub-structure

Yield

Record Type

Reagent/Catalyst

Solvent

Reaction Type

No. of Steps

Product Availability

Reactant Availability

Availability in other DBs

Molecular Weight

Number of Fragments

Physical Data

226 reactions out of 334 substances and 208 citations

Reactions

Substances (Grid)

Substances (Table)

Citations

Limit to

Exclude

Output

Print

Zoom in

Zoom out

Hide

Sort by

Reaxys-RXID

Number of References

Reactant Availability

Product Availability

MW of product

Publication Year

Yield

Reaxys-Ranking

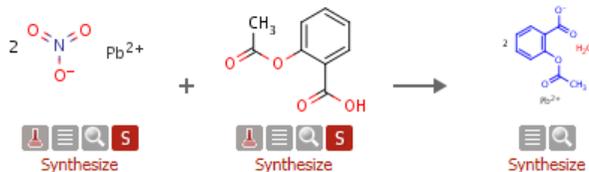
go to Page



Page 1 of 26



1



Rx-ID: 35472532

Find similar reactions

92%

Stage #1: Aspirin With sodium hydroxide in ethanol; water
T=0 - 20°C; pH=9; 1 h;
Stage #2: lead (II) nitrate in ethanol; water
T=0 - 20°C; 25 h;

Show Experimental Procedure

De Jesus Palacios-Hernandez, Teresa; Vasquez-Arciga, Horacio; Perez-Benitez, Aaron; Bernes, Sylvain; Hoepfl, Herbert; Gonzalez-Vergara, Enrique; Mendez-Rojas, Miguel Angel

Polyhedron, 2013, vol. 52, p. 848 - 855

Title/Abstract

Full Text

View citing articles

Show Details



Reactions **Substances (Grid)** Substances (Table) Citations go to Page Page 1 of 38

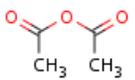
Limit to Exclude Output Print Zoom in

Sort by No of References

226 reactions out of 334 substances and 208 citations

Reactions **Substances (Grid)** **Substances (Table)** Citations go to Page Page 1 of 38

Limit to Exclude Output Print Zoom in Zoom out Hide Sort by No of References

Structure	Structure/Compound Data	N° of preparations All Preps All Reactions	Available Data	N° of ref.
 1 Synthesize	Chemical Name: acetic anhydride Reaxys Registry Number: 385737 CAS Registry Number: 108-24-7 Type of Substance: acyclicIsotope or isotope containing compound Molecular Formula: C ₄ H ₈ O ₃ Linear Structure Formula: O(COCH ₃) ₂ Molecular Weight: 102.09 InChI Key: WFDJRYMOXRFFG-UHFFFAOYSA-N	497 prep out of 190645 reactions.	Identification Physical Data (454) Spectra (71) Bioactivity (16) Use/Application (16) Natural Product (7)	98437
 2 Synthesize Show Details	Chemical Name: water Reaxys Registry Number: 3587155 CAS Registry Number: 7732-18-5 Type of Substance: Isotope or isotope containing compoundGlass or Ceramic materialCoordination compound Molecular Formula: H ₂ O Linear Structure Formula: (¹ H) ₂ O Molecular Weight: 18.0153 InChI Key: XLYOFNOQVPJJNP-UHFFFAOYSA-N	5146 prep out of 98075 reactions.	Identification Physical Data (14266) Spectra (1394) Bioactivity (53) Use/Application (1795) Quantum Chemical Data (1462)	85194
 3 Synthesize	Chemical Name: acetic acid Reaxys Registry Number: 506007 CAS Registry Number: 64-19-7 Type of Substance: acyclic	4619 prep out of 72635 reactions.	Identification Physical Data (4654) Spectra (439) Bioactivity (367) Ecological Data (131) Use/Application (922)	48231

Identification
Physical Data (454)
Spectra (71)
Bioactivity (16)
Use/Application (16)
Natural Product (7)

Identification
Physical Data (10260)
Spectra (883)
Bioactivity (575)
Ecological Data (810)



记录该反应的详细文献题录信息

226 reactions out of 334 substances and 208 citations

Reactions Substances (Grid) Substances (Table) Citations

Limit to Exclude Output Print Zoom in Zoom out Hide Sort by Relevance

	Title of the Document	Authors	Year	Source	Times cited
<input type="checkbox"/>	Substituted bis-hydroxyphenyl pentanes	Ciba-Geigy Corporation	1976	Patent: US3956402 A1, 1976 ; Patent Family: US3956402 A1; Full Text	
	▼ Title/Abstract ▼ Front page Information ▼ Show All Reactions (4) ▼ Hit Reactions in this article (1 out of 4) ▼ Show All Substances (7)				
<input type="checkbox"/>	Alkylphenols	Ciba-Geigy Corporation	1976	Patent: US3991124 A1, 1976 ; Patent Family: US3991124 A1; Full Text	
	▼ Title/Abstract ▼ Front page Information ▼ Show All Reactions (5) ▼ Hit Reactions in this article (1 out of 5) ▼ Show All Substances (7)				
<input type="checkbox"/>	Benzothienyl anketones and the application in th				

Show All Reactions: 显示该文献中的所有化学反应信息

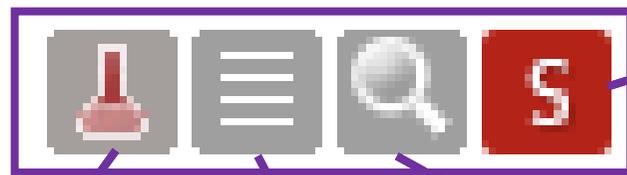
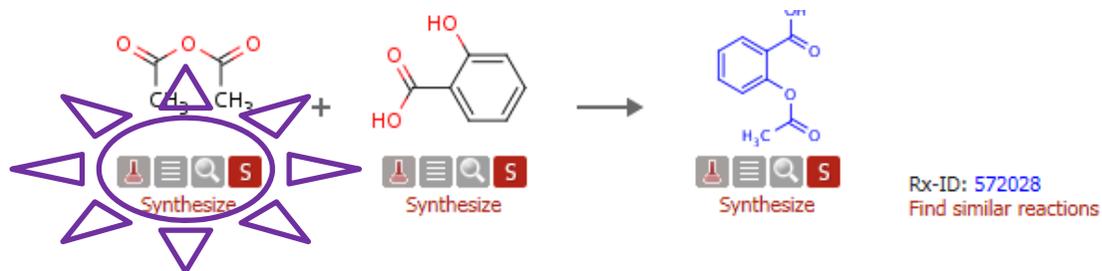
Hit Reactions in this article: 只显示该文献中与检索条件匹配的化学反应

Show All Substances: 显示该文献中所有的化学物质

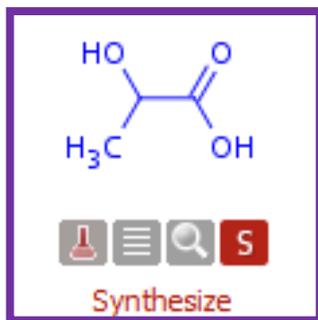


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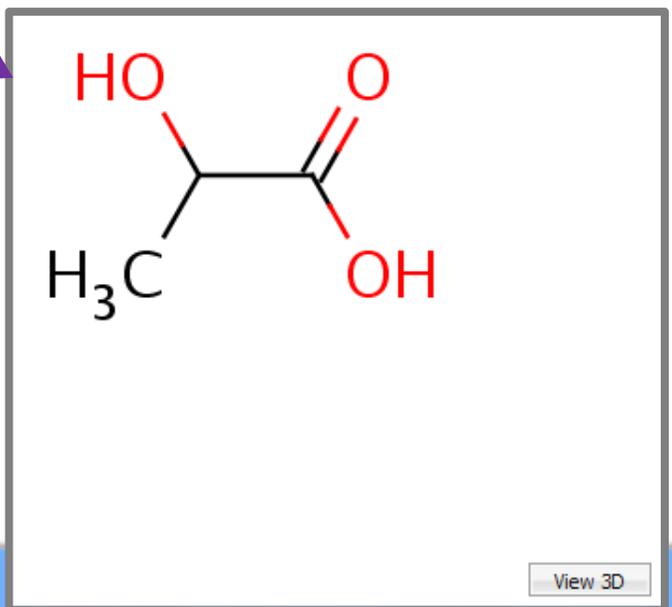


Show corresponding substances in...
PubChem
eMolecules



Available through...
Accelrys' ACD
2500g
\$107 eMolecules
CambridgeSoft ACX
Safety Data...
PharmaPendium

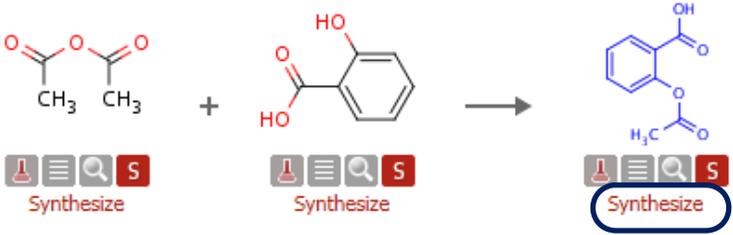
Reaxys-RN: 1209341
MF: C3H6O3
MW: 90.0788
CAS-RN: 849585-22-4
Show Details
Copy Structure to Clipboard
Copy Structure to Query
Use as Substructure Filter
Copy Reaction to Query
View related Markush





Synthesis Plans: 设计合成路线图

4



Manually
by Autoplan
by Autoplan (with options)

Rx-ID: 572028
Find similar reactions

99%	With erbium(III) chloride 0.2 h; Heating;	Dalpozzo, Renato; De Nino, Antonio; Maiuolo, Loredana; Oliverio, Manuela; Procopio, Antonio; Russo, Beatrice; Tocci, Amedeo Australian Journal of Chemistry, 2007 , vol. 60, # 1 p. 75 - 79 Title/Abstract Full Text View citing articles Show Details
95%	With nano-crystalline sulfated zirconia T=120°C; 0.5 h;	Tyagi, Beena; Mishra, Manish Kumar; Jasra, Raksh Vir Journal of Molecular Catalysis A: Chemical, 2010 , vol. 317, # 1-2 p. 41 - 45 Title/Abstract Full Text View citing articles Show Details
95%	With sulfuric acid 2 h; Reflux;	Xiong, Lin; Gao, Ya-Qin; Niu, Chu-E.; Wang, Hong-Bo; Li, Wei-Hong Letters in Drug Design and Discovery, 2014 , vol. 11, # 2 p. 132 - 137 Title/Abstract Full Text View citing articles Show Details

[Show Next 20 Details](#)

Qry
His
Rep



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Query Results **Synthesis Plans** History Report My Alerts My Settings Help Logout

Synthesis 1

New Undo Open Save Rename Duplicate Output Print LeRt Right Top Resize Thumbnail Report Hide

Hints

- Click on "Synthesize" to find all preparations of the compound.
- In the browser below review the preparations and "Add" the best one to the synthesis tree.
- "Add" a branch or click on the button "Duplicate" if you want to investigate alternative routes.

CH₃ C(=O)O C(=O)CH₃

Synthesize (457)

1 Details 99% Add Remove

Manually by Autoplan

HO C(=O)C₆H₄CO₂H

Synthesize (623)

Manually by Autoplan (with)

Zoom in Zoom out Hide Sort by Reaxys-Ranking

Yield	Conditions	References
92%	With iron sulphate heptahydrate; Oxonereg; in water T=20°C; 0.5 h; Sonication; Green chemistry; Show Experimental Procedure	Mirza-Aghayan, Maryam; Molaee Tavana, Mahdieh; Boukherroub, Rabah Tetrahedron Letters, 2014 , vol. 55, # 2 p. 342 - 345 Title/Abstract Full Text View citing articles Show Details
88%	With C ₃₀ H ₂₄ AgBr ₄ N ₈ (¹⁺) ₂ AgBr ₂ (¹⁻); potassium hydroxide in ethylene glycol dimethyl ether T=60°C; 24 h; Molecular sieve; Schlenk technique;	Han, Lei; Xing, Ping; Jiang, Biao Organic Letters, 2014 , vol. 16, # 13 p. 3428 - 3431 Title/Abstract Full Text View citing articles Show Details
86%	With sodium tetrahydroborate; 1 Pd/C; water; potassium hydroxide in methanol T=20°C; 24 h; In air;	An, Gwangil; Ahn, Hyunseok; De Castro, Kathlia A.; Rhee, Hakjune Synthesis, 2010 , # 3 art. no. F1900955, p. 477 - 485 Title/Abstract Full Text View citing articles Show Details

▼ Show All Remaining Details (3)

HO C(=O)C₆H₄CO₂H

HO C(=O)C₆H₄CO₂H

Add selected Create new plan Rx-ID: 280761

Add selected Create new plan Rx-ID: 827728

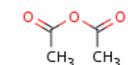


Report

Query Results Synthesis Plans History **Report** My Alerts My Settings Help

Synthesis 1

New Undo Open Save Rename Duplicate Output Print Left Right Top Resize Thumbnail **Report** Show



Synthesize (457)

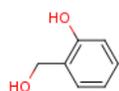
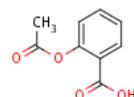


1

Details

99 %

Add



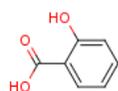
2

Details

92 %

Add Remove

Synthesize (148)



2

92 %



1

99 %

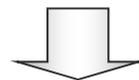


Hide Synthesis Details

Step	Yield	Conditions	References
1 Reaxys	99%	With erbium(III) chloride 0.2 h; Heating;	Dalpozzo, Renato; De Nino, Antonio; Maiuolo, Loredana; Oliverio, Manuela; Procopio, Antonio; Russo, Beatrice; Tocci, Amedeo Australian Journal of Chemistry, 2007, vol. 60, # 1 p. 75 - 79 Title/Abstract Full Text View citing articles Show Details
	95%	With nano-crystalline sulfated zirconia T=120°C; 0.5 h;	Tyagi, Beena; Mishra, Manish Kumar; Jasra, Raksh Vir Journal of Molecular Catalysis A: Chemical, 2010, vol. 317, # 1-2 p. 41 - 45 Title/Abstract Full Text View citing articles Show Details
	95%	With sulfuric acid 2 h; Reflux;	Xiong, Lin; Gao, Ya-Qin; Niu, Chu-E.; Wang, Hong-Bo; Li, Wei-Hong Letters in Drug Design and Discovery, 2014, vol. 11, # 2 p. 132 - 137 Title/Abstract Full Text View citing articles Show Details



检索吸入时有平喘疗效的化合物

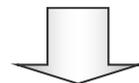


检索示例2:
物质检索

化合物

疗效: 平
喘

用法: 吸
入



通过物质的药理学性质
查找合适的化合物



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Reactions **Substances** Literature

Structure

selected query editor: MarvinSketch by ChemAxon

Available to add | Already selected | Searches in multiple databases

Insert/Remove Properties

Define the "Substances" query layout

Find any property

- [-] Catalyst Investigation exists
- [+] Derivative exists
- [+] Purification exists
- [+] Physical Data
- [+] Spectra
- [-] Bioactivity
 - [-] Pharmacological Data exists
 - Effect (PHARM.E)
 - Endpoint of Effect (PHARM.EP)
 - Species or Test-System (PHARM.SP)
 - Sex (PHARM.S)
 - Route of Application (PHARM.RA)
 - Concentration (PHARM.C)
 - Kind of Dosing (PHARM.KD)

Reaxys Registry Number (in multiple)
CAS Registry Number (in Reaxys)
Chemical Name (in multiple)
Element Symbols (in multiple)

Identification

Reaxys Registry Number = Lookup X

CAS Registry Number is Lookup X

Chemical Name is Lookup X

Element Symbols is Lookup X

Show AND Buttons

Add to Query: Structure Molecular Formula Alloy **Add/Remove Fields...** Search Substances



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Insert/Remove Properties

Define the "Substance"

Find any property

Category:

- Deriva
- Purific
- Physical De
- Spectra
- Bioactivity
 - Pharm
 - Effect
 - Endp
 - Speci
 - Sex (
 - Route
 - Conc
 - Kind

Available to add

Structure

selected query editor:



Create Structure Template from Name

As drawn
 Substructure
 on heteroatoms
 on all atoms
 Similarity

Include tautomers
 Ignore stereo
 No salts
 No mixtures
 No isotopes
 No charges
 No radicals
 No ring closures
 Align results with query

[More options](#)

Identification

Reaxys Registry Number	=	<input type="text"/>	Lookup	×
CAS Registry Number	is	<input type="text"/>	Lookup	×
Chemical Name	is	<input type="text"/>	Lookup	×
Element Symbols	is	<input type="text"/>	Lookup	×

Show AND Buttons

Bioactivity

Effect	is	<input type="text" value="antiasthma"/> 平喘	Lookup	×
Route of Application	is	<input type="text" value="inhalation"/> 吸入	Lookup	×

Show AND Buttons

Add to Query: [Structure](#) [Molecular Formula](#) [Alloy](#) [Add/Remove Fields...](#)

Search Substances



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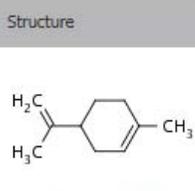
该物质参与化学反应的信息

26 substances out of 1907 reactions and 4811 citations

Filter by:

- Sub-structure
- Molecular Weight
- Number of Fragments
- Physical Data
- Spectroscopic Data
- Bioactivity
- Ecological Data
- Natural Product
- Availability
- Availability in other DBs

Reactions Substances (Grid) **Substances (Table)** Citations



Chemical Name:
p-mentha-1,8-diene
Reaxys Registry Number: 774123
CAS Registry Number: 138-86-3
Type of Substance: isocyclic
Molecular Formula: C₁₀H₁₆
Linear Structure Formula: CH₃C₆H₈C(CH₂)CH₃
Molecular Weight:
InChI Key: XMGQY...

N° of preparations
All Preps | All Reactions
330 prep
out of
755 reactions.

Available Data
Hit Data (1)
Identification
Physical Data (463)
Spectra (79)
Bioactivity (253)
Ecological Data (74)
Use/Application (150)
Natural Product (310)

N° of ref.
1516

有关该物质的基本信息

Chemical Names and Synonyms

p-mentha-1,8-diene, Limonene, (±)-limonene, p-menth-1,8-diene, α-limonene, dl-limonene, Dipentene

- Hit Data
- Identification
- Physical Data
- Spectra
- Bioactivity
- Pharmacological Data (197)
- Ecotoxicology (56)
- Ecological Data
- Use/Application

可获取数据内容

Hit Data: 与查询条件相匹配的数据记录



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Chemical Names and Synonyms

p-mentha-1,8-diene, Limonene, (±)-limonene, p-menth-1,8-diene, α-limonene, dl-limonene, Dipent

Hit Data

Pharmacological Data (1 Hits out of 197 view all)

1 of 1	Effect	antiasthma
	Species or Test-System	Brown Norway rat
	Sex	male
	Route of Application	inhalation
	Concentration	125 ppm
	Kind of Dosing	in air; animals breathed continuously
	Method	4-week-old rats sensitized on d 0; received title comp.; Penh value measured
	Further Details	OVA: ovalbumin; sensitization by: heat killed organisms in saline; non
	Results	title comp. treatment resulted in significant decrease in Penh values close to that in control (1.71 and 1.70, resp.) in comparison with non-treated sensitized rats (2.34); after title comp. treatment minimal to mild pathological changes in lungs found
	Reference	Keinan, Ehud; Alt, Aaron; Amir, Gail; Bentur, Lea; Bibi, Haim; Shoseyov, David <i>Bioorganic and Medicinal Chemistry</i> , 2005, vol. 13, # 2, p. 557-562
		Title/Abstract Full Text View citing articles Show Details

每条记录都有对浓度、用量、使用方法以及效果等方面的详细数据

Title/Abstract: 超链接访问文献记录

Full Text: 链接到文献全文

View citing articles: 链接到Scopus数据库中的该文献记录, 查看该文献被引用情况

Show Details: 详细的文献题录信息



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- Physical Data
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- Availability
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- Yield
- Record Type
- Reagent/Catalyst
- Solvent
- Reaction Type
- No. of Steps
- Product Availability
- Reactant Availability
- Availability in other DBs
- Document Type
- Authors

Reactions Substances (Grid) **Substances (Table)** Citations

Limit to Exclude **Output** Print Zoom in Zoom out Hide

Sort by No of References

Structure

Synthesize | Hide Details

Chemical Names and Descriptions
p-mentha-1,8-diene

Hit Data

Identification

Physical Data

Spectra

Bioactivity

Pharmacology

Ecotoxicology

Ecological Data

Use/Applications

检索结果的导出

Reaxys: Output Reaction Results

Output to

- Substances Grid
- Substances Details Table
- Substances Reactions Table
- Substances Citations Table

PDF/Print options:

- PDF/Print
- XML
- Microsoft Word
- Microsoft Excel
- Literature Management Systems (e.g. ReferenceManager, EndNote etc.)
- RD File

Include the following headline

Output range

- All hits
- Range: e.g. 1, 2-5, 10

Output contains

- Include structures
- Include experimental procedure
- All available data
- Identification data only
- Hit data only

OK Cancel

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功能：实验步骤、全文、精炼、合成路线设计

提供经过确认的可靠的实验数据

- 科研杂志——物化数据；生物活性；自然产物；反应产率，反应条件，反应物/溶剂；催化剂；商品等；
- 专利——实验过程和光谱信息数据(NMR; IR; MS; UV/VIS)。

化学反应路线合成：

- 设计多步骤反应，比较可供选择的反应路线，帮您做出快速而准确的判断。

Reaxys排序，过滤和分析工具：

- 很容易找到、过滤和分析所得到数据，效率很高。

轻松访问：

- 总是能找到您所需要的信息。





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谢谢!