



Conozca Reaxys



Reaxys

Reaxys es la nueva herramienta de Elsevier desarrollada especialmente para investigadores de las áreas de química, bioquímica y farmacología.

Reaxys promueve la descubierta y la innovación integrando la investigación de propiedades de sustancias y reacciones con la planificación de síntesis químicas.

- Consulte procedimientos experimentales y rendimientos de reacciones químicas en segundos
- Analice las propiedades físicas, farmacéuticas y de toxicidad de los compuestos extraídas de los artículos científicos y de patentes
- Desarrolle la mejor estrategia de síntesis con la exclusiva herramienta de síntesis de Reaxys



Reaxys - Contenido

Reaxys reúne el contenido más relevante de la literatura científica y de patentes en química orgánica, inorgánica y órgano metálica a través de las consagradas bases de datos

- **CrossFire Beilstein** – química orgánica
- **CrossFire Gmelin** – química inorgánica y órgano metálica
- **Patent Chemistry Database**



Facilidad de búsqueda

The screenshot displays the Reaxys search interface. At the top left is the Reaxys logo. A navigation bar contains links for Query, Results, Synthesis Plans, History, My Settings, Help, Register, and Login. Below this, there are tabs for Reactions, Substances and Properties, and Text, Authors and more. A search box labeled 'Generate structure from name' is present, with a red arrow pointing to it. Below the search box is a large empty frame with the instruction 'Double click this frame and draw reaction query'. To the right of the search box are two panels of search options. The first panel, 'Search as / by', has radio buttons for Product (selected), Starting material, Any role, Reagent/ Catalyst, As drawn (selected), and Substructure: (with sub-options for on heteroatoms and on all atoms). The second panel has checkboxes for Ignore stereo, No isotopes, No charges, No radicals, No additional rings, Keep Fragments separate, and Ignore Atom Mappings. A 'Search' button is located at the bottom right. A modal dialog box is open, titled 'Please enter a chemical identifier and then click "Submit"', with a text input field containing 'aspirin'. Below the input field are three example identifiers: 'Example 1: aspirin', 'Example 2: BSYNRYMUTXBXSQ-WXRBYKJCCW', and 'Example 3: 50-78-2'. The dialog has 'Submit' and 'Cancel' buttons. At the bottom of the interface are 'Clear Query', 'Load Query', and 'Save Query' buttons, and a footer with contact information and copyright notice.

reaxys

Query Results Synthesis Plans History My Settings Help Register Login

Reactions Substances and Properties Text, Authors and more

Generate structure from name

Double click this frame and draw reaction query

Please enter a chemical identifier and then click "Submit"

aspirin

Example 1: aspirin
Example 2: BSYNRYMUTXBXSQ-WXRBYKJCCW
Example 3: 50-78-2

Submit Cancel

Search as / by

Product
 Starting material
 Any role
 Reagent/ Catalyst
 As drawn
 Substructure:
 on heteroatoms
 on all atoms

Ignore stereo
 No isotopes
 No charges
 No radicals
 No additional rings
 Keep Fragments separate
 Ignore Atom Mappings

Add further search conditions

Search

Clear Query Load Query Save Query

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Interfaz intuitiva: búsquedas por nombre, diseño del compuesto o reacción, número CAS o InChi-Key

Recursos inteligentes para filtrar y ordenar resultados

Query Results Synthesis Plans History My Settings Help Logout

Query 24 reactions 2 reactions Limited by hits

Ordene los resultados por:
- Reaxys-Ranking: reacciones más detalladas
- Reacciones de mayor rendimiento

2 reactions out of 4 citations go to Page Page 1 of 1

Filter by:
Yield
Record Type
Reagent/Catalyst
Solvent
Reaction Type
No. of Steps
Document Type
Authors
Patent Assignee
Journal Title
Publication Year

Reactions Citations

Limit to Selection Output Sort by Reaxys-Ranking

Yield Conditions References

1

Product commercially available
Enlace para informaciones comerciales

Rx-ID: 8619391

243.3 g With aq. hydrazine hydrate in tetrahydrofuran; methanol T=10 - 20°C; Reduction cyclization; Katayama, Masato Bioscience, Biotechnology, and Biochemistry, 2000, vol. 64, # 4 p. 808 - 815 Title/Abstract Full Text Scopus

74% With Zn; AcOH in methanol; CH₂Cl₂ Heating; Siu, Jason; Baxendale, Ian R.; Ley, Steven V. Organic and Biomolecular Chemistry, 2004, vol. 2, # 2 p. 160 - 167 Title/Abstract Full Text Scopus

in benzene 969212; Show Experimental Procedure Hoffmann-La Roche Inc. Patent: US3976639, 1976 Title/Abstract Full Text

2

Filtros para los resultados

Rx-ID: 18555314

Multi-step reaction with 2 steps
1: 1.) Triton B, 2.) Zn, CaCl₂ / 1.) Me₂SO, 95 deg C, 1 h, 2.) H₂O, reflux
2: 92 percent / RuCl₂(PPh₃)₃ / toluene / 6 h / Heating
View Scheme

Tsuji, Yasushi; Huh, Keun-Tae; Yokoyama, Yasuharu; Watanabe, Yoshihisa
Journal of the Chemical Society, Chemical Communications, 1986, # 21 p. 1575 - 1576
Title/Abstract Full Text Scopus

Recursos inteligentes para filtrar y ordenar resultados

Filter by:

Yield

<input type="checkbox"/> >95 - 100	2
<input type="checkbox"/> >85 - 90	1
<input type="checkbox"/> >75 - 80	4
<input type="checkbox"/> >70 - 75	1

More

Limit to Exclude

Record Type

<input type="checkbox"/> full reaction	162
<input type="checkbox"/> has preparation	118
<input type="checkbox"/> half reaction	26
<input type="checkbox"/> has multi-step	1

Limit to Exclude

Reagent/Catalyst

<input type="checkbox"/> water	13
<input type="checkbox"/> 10 percent human plasma	12
<input type="checkbox"/> oh-	9
<input type="checkbox"/> methanol	9

More

Limit to Exclude

Solvent

<input type="checkbox"/> h2o	32
<input type="checkbox"/> acetonitrile	20
<input type="checkbox"/> methanol	18
<input type="checkbox"/> dioxane	18

More

Limit to Exclude

Reaction Type

<input type="checkbox"/> hydrolysis	2
<input type="checkbox"/> complexation	2
<input type="checkbox"/> substitution	1
<input type="checkbox"/> acetylation	1

More

Limit to Exclude

No. of Steps

<input type="checkbox"/> 1	187
<input type="checkbox"/> 2	1

Limit to Exclude

Document Type

<input type="checkbox"/> journal	108
<input type="checkbox"/> patent	58
<input type="checkbox"/> book review / secondary ref.	2

Limit to Exclude

Authors

<input type="checkbox"/> abordo, evelyn a.	1
<input type="checkbox"/> aboul-fadl, tarek	1
<input type="checkbox"/> abraham j.	1
<input type="checkbox"/> abuhijleh, a. latif	1

More

Limit to Exclude

Patent Assignee

<input type="checkbox"/> abraham j.	1
<input type="checkbox"/> alfatec-pharma gmbh	1
<input type="checkbox"/> antognazza, patrizia	1
<input type="checkbox"/> ashton, paul	1

More

Limit to Exclude

Journal Title

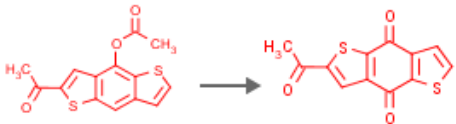
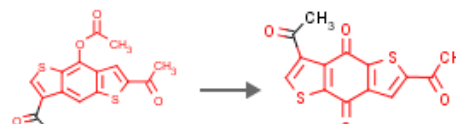
Publication Year



La mejor fuente para investigar reacciones químicas

Reactions Citations

Limit to Selection Output Sort by

Yield	Conditions	
<input type="checkbox"/> 1  <p>Rx-ID: 5168182</p>	<p>With HOAc, CrO₃ 1 h; Yield given;</p> <p>45% With chromium(VI) oxide in acetic acid 1 h; 10773376; 506007; Hide Experimental Procedure</p>	<p>Chao, Yu-Hua; Kuo, Sheng-Chu; Wu, Chun-Hsiung; Lee, Chun-Yann; Mauger, Anthony; et al. Journal of Medicinal Chemistry, 1998, vol. 41, # 23 p. 4658 - 4661 Title/Abstract Full Text Scopus</p> <p>University of North Carolina at Chapel Hill Patent: US6337346, 2002 Title/Abstract Full Text</p>
<p>Example 1 2-Acetyl-4,8-dihydrobenzo[1,2-b:4,5-b']dithiophene-4,8-dione (9) To a stirring mixture of acetyl chloride (5.1 g, 65 mmol) and AlCl₃ (8.7 g, 65 mmol) in 1,2-dichloroethane (200 ML) under N₂ was added dropwise a solution of 4-acetoxybenzo[1,2-b:4,5-b']dithiophene (7)7a (8 g, 32.3 mmol) in 1,2-dichloroethane (90 ML).. After stirring for 4 h, this solution was poured into dilute HCl and the aqueous layer was extracted with CHCl₃ three times.. The combined extracts were washed with saturated NaHCO₃ and water, dried over anhydrous MgSO₄, and concentrated under reduced pressure to give 7.5 g of the crude intermediate 4-acetoxy-2-acetylbenzo[1,2-b:4,5-b']dithiophene (8). To a suspension of crude 8 (7.5 g) in HOAc (30 ML) was added CrO₃ (5.7 g, 57 mmol).. After stirring for 1 h, i-PrOH (20 ML) and CHCl₃ (300 ML) were added and stirred for 30 min.. The resulting solution was poured into ice water, and the aqueous layer was extracted with CHCl₃ three times.. The combined extracts were dried over anhydrous MgSO₄ and concentrated under reduced pressure.. The residue was purified by column chromatography (silica gel, CHCl₃) to give 9 (mp 223-225 .deg. C.) in a 45percent yield. IR (KBr) 1650, 1670 (C=O) cm⁻¹; ¹H NMR (CDCl₃) δ 2.67 (s, 3H, CH₃), 7.68 (d, J=5.1 Hz, 1H, H-7), 7.74 (d, J=5.1 Hz, 1H, H-6), 8.12 (s, 1H, H-3); ¹³C NMR (CDCl₃): δ 26.9 (C-2-CH₃), 126.9 (C-7), 129.4 (C-3), 134.3 (C-6), 170.0 (C-4), 174.4 (C-8), 190.7 (C-2-C=O); MS m/z 262 (M⁺); Anal. (C₁₂H₆O₃S₂) C, H.</p>		
<input type="checkbox"/> 2 		

1. Reacciones similares, pero con condiciones diferentes son extraídas de diversos artículos científicos y patentes y después reunidas en una única tabla
2. Los textos con procedimientos de reacciones patentadas son exhibidos para inmediata validación de las condiciones

De un artículo científico

De una patente

1
2

Reaxys - Microsoft Internet Explorer
Internet

Beneficios para la química medicinal

Evite procedimientos de laboratorio dispendiosos para a validación de datos calculados

- Reaxys contiene datos experimentales extraídos de la literatura científica:
- Puntos de fusión / ebullición, solubilidad
- Coeficiente de partición octanol/water logP
- Constantes de disociación pKa

Datos de bioactividad y toxicidad, por ejemplo:

- Inhibición / concentración efectiva (e.g. IC/EC50)
- Constantes de unión / disociación (K_i/k_d)

Evite el trabajo de coleta manual de informaciones usando el recurso “Substance Profiles“ y obtenga todos los datos de una sustancia en un único registro



Evite procedimientos de laboratorio dispendiosos

Substances (Grid) Substances (Table) Citations 1 substances out of 480 citations go to No. Page 1

Limit to Selection Sort by Molweight

Structure	Chemical Name	Available Data
	5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)-methyl]sulphonyl]-1H-benzimidazole (-)-5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methyl]sulfinyl]-1H-benzimidazole 5-methoxy-2-[[4-methoxy-3,5-dimethyl-2-pyridyl)methylsulphonyl]-1H-benzimidazole 5-methoxy-2-[[4-methoxy-3,5-dimethyl-pyridin-2-yl)-methylsulfinyl]benzimidazole 2-[[3,5-dimethyl-4-methoxypyridin-2-yl)methylsulfinyl]-5-methoxybenzimidazole rac-omeprazole	Identification (70) Physical Data (41) Spectra (26) Bioactivity/ECotox (658) Use/Application (746)

Structure/Compound Data

Reaxys Registry Number: 3628192
CAS Registry Number: 73590-58-6 119141-88-7 119141-89-8 131959-78-9 326602-80-6
Chemical Name: 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)-methyl]sulphonyl]-1H-benzimidazole, (-)-5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridinyl)methyl]sulfinyl]-1H-benzimidazole, 5-methoxy-2-[[[(4-methoxy-3,5-dimethyl-2-pyridyl)methyl]sulfinyl]-1H-benzimidazole, 5-methoxy-2-[[4-methoxy-3,5-dimethyl-2-pyridyl)methylsulphonyl]-1H-benzimidazole, 5-methoxy-2-[[4-methoxy-3,5-dimethyl-pyridin-2-yl)-methylsulfinyl]benzimidazole, 2-[[3,5-dimethyl-4-methoxypyridin-2-yl)methylsulfinyl]-5-methoxybenzimidazole, rac-omeprazole
Type of Substance: heterocyclic

Molecular Formula: C₁₇H₁₉N₃O₅S
Linear Structure Formula: C₁₇H₁₉SN₃O₅
Molecular Weight: 345.422
InChi Key: SUBDBMMJZJVS-LILDPLRNC

Pharmacological Data (797)

Effect	Species or Test-System	Sex	Route of Application	Concentration	Method	Further Details	Type	Value of Type	Results	Comment	Reference
enzyme activity; inhibition of	recombinant aldo-keto reductase 1C1				enzyme incubated with title comp.; enzyme activity determined using 9,10-phenanthrene quinone substrate	1C1: 20α-hydroxysteroid dehydrogenase	IC50	29 μmol/l			Byrns, Michael C.; Steckelbroeck, Stephan; Penning, Trevor M. Biochemical Pharmacology, 2008, vol. 75, # 2 p. 484-493 Title/Abstract Full Text Scopus

Valores experimentales para:

- Solubilidad
- Coeficiente de partición octanol/water logP
- Exponente de disociación pK_a
- Datos de bioactividad (ex: IC/EC, Ki/Kd)
- Datos toxicológicos

Datos farmacológicos (bio-ensayos)

Type	Value of Type
IC50	29 μmol/l

Propiedades experimentales

Ejemplos de datos experimentales encontrados para un compuesto buscado:

▼ Identification	▼ Enthalpy of Vaporization (1)	▲ Spectra
▲ Physical Data	▼ Heat Capacity Cp (1)	▼ NMR Spectroscopy (16)
▼ Melting Point (5)	▼ Other Thermochemical Data (3)	▼ IR Spectroscopy (3)
▼ Boiling Point (17)	▼ Electrochemical Behaviour (5)	▼ Mass Spectrometry (4)
▼ Refractive Index (8)	▼ Dissociation Exponent (5)	▼ Raman Spectroscopy (1)
▼ Density of the Liquid (7)	▼ Further Information (1)	▼ Other Spectroscopic Methods (1)
▼ Conformation (1)	▼ Solubility (MCS) (1)	▼ Bioactivity/ECOTOX
▼ Electrical Moment (2)	▼ Liquid/Vapour Systems (MCS) (2)	▲ Use/Application
▼ Ionization Potential (1)	▼ Azeotropes (MCS) (1)	▼ Use (1)
▼ Vapour Pressure (1)	▼ Liquid/Liquid Systems (MCS) (9)	▲ Natural Product
▼ Mechanical Properties (1)	▼ Mechanical & Physical Properties (MCS) (2)	▼ Derivative (23)
▼ Transport Data (1)	▼ Transport Phenomena (MCS) (1)	▼ Purification (1)
	▼ Energy Data (MCS) (4)	
	▼ Association (MCS) (12)	



Los números representan el número de resultados encontrados en esta búsqueda para cada propiedad



Propiedades experimentales

Ejemplos de datos experimentales encontrados para un compuesto buscado:

▲ NMR Spectroscopy (22)

Description	Nucleus	Solvents	Frequency	Original Text	Reference
CPMAS (Cross Polarization Magic-Angle Spinning) Solid phase	¹³ C			20.5+/-0.5 ppm; 19.8 (+/-0.5 ppm) ppm	SCICONCEPT GMBH Patent: WO2008/37289 , 2008 Title/Abstract Full Text
CPMAS (Cross Polarization Magic-Angle Spinning) Solid phase	¹³ C				SCICONCEPT GMBH Patent: WO2008/37289 , 2008 Title/Abstract Full Text
Chemical shifts	¹ H	CDCl ₃	300MHz		Rastrelli, Federico; Bagno, Alessandro Journal of Magnetic Resonance, 2006 , vol. 182, # 1 p. 29 - 37 Title/Abstract Full Text Scopus
	¹ H	CDCl ₃		¹ H NMR (CDCl ₃), 2.37 (s, 3H), 5.83 (s, 2H), 7.12 (m, 1H), 7.34 (m, 1H), 7.62 (m, 1H), 7.72 (d, 2H), 8.05 (dd, 1H)	Ashton, Paul; Cynkowska, Grazyna; Cynkowski, Tadeusz; Smith, Thomas J. Patent: US2003/170286 , 2003 Title/Abstract Full Text Control Deliver Systems, Inc. Patent: US2005/164994 , 2005 Title/Abstract Full Text
	¹ H	CDCl ₃		¹ H NMR (CDCl ₃): 8.21 (1H,dd); 7.66 (1H,dt); 7.42 (3H,m); 7.20 (3H,m); 5.40 (2H, s), 2.25 (3H,s)	Del Soldato, Piero Patent: US2004/23890 , 2004 Title/Abstract Full Text
	¹ H		200MHz	¹ H NMR (200 MHz) (CDCl ₃): 8.10 (2H, m); 7.7 (1H, t); 7.56(2H, d); 7.48 (1H, t); 7.30(1H, d); 5.74 (2H, s); 5.43 (2H, s); 2.20 (3H, s)	Del Soldato, Piero; Benedini, Francesca; Antognazza, Patrizia Patent: US2004/23933 , 2004 Title/Abstract Full Text
Spectrum	¹ H	tetradeuteriomethanol			Leo, Gregory C.; Krikava, Aaron; Caldwell, Gary W. Analytical Chemistry, 2003 , vol. 75, # 8 p. 1954 - 1957 Title/Abstract Full Text Scopus

Propiedades experimentales

Ejemplos de datos experimentales encontrados para un compuesto buscado:

▲ Pharmacological Data (1775)									
Effect	Species or Test-System	Sex	Route of Application	Concentration	Method	Type	Value of Type	Results	Reference
protein expression; effect on	umbilical vein endothelial cells of human			2.5 - 5 mmol/l	cells treated with 100 or 300 µg/ml ox-LDL for 16 h; cells pre-incubated with title comp. for 30 min; effect of title comp. on COX-2 expression induced by ox-LDL			cells pre-incubated with title comp. signif. reduced COX-2 expression induced by ox-LDL; fig.	Zhao, Jinjing; Qi, Ruomei; Li, Rui; Wu, Wei; Gao, Xin; Bao, Li; Lu, Shuzheng Journal of Cardiovascular Pharmacology, 2008 , vol. 51, # 1 p. 32 - 37 Title/Abstract Full Text Scopus
protein expression; effect on	umbilical vein endothelial cells of human			2.5 - 5 mmol/l	cells treated with 100 or 300 µg/ml ox-LDL for 16 h; cells pre-incubated with title comp. for 30 min; effect of title comp. on ICAM-1 expression induced by ox-LDL			title comp. almost completely suppressed ICAM-1 expression induced by ox-LDL; title comp. alone had no effect on ICAM-1 expression in unstimulated cells; fig.	Zhao, Jinjing; Qi, Ruomei; Li, Rui; Wu, Wei; Gao, Xin; Bao, Li; Lu, Shuzheng Journal of Cardiovascular Pharmacology, 2008 , vol. 51, # 1 p. 32 - 37 Title/Abstract Full Text Scopus
protein expression; effect on	umbilical vein endothelial cells of human			2.5 - 5 mmol/l	cells treated with 100 or 300 µg/ml ox-LDL for 16 h; cells pre-incubated with title comp. for 30 min; effect of title comp. on ICAM-1 expression induced by ox-LDL detd. by using western blot			title comp. almost completely suppressed ICAM-1 expression induced by ox-LDL; fig.	Zhao, Jinjing; Qi, Ruomei; Li, Rui; Wu, Wei; Gao, Xin; Bao, Li; Lu, Shuzheng Journal of Cardiovascular Pharmacology, 2008 , vol. 51, # 1 p. 32 - 37 Title/Abstract Full Text Scopus

Beneficios para los químicos medicinales

Actividad

Encontrar sustancias con determinadas propiedades o drogas con ciertos efectos

Comprender los efectos de una droga e interacciones droga-objetivo biológico

Analizar resultados de búsquedas para encontrar nuevas sustancias con estructuras similares

Encontrar sustancias separadas de los productos naturales

Beneficios de Reaxys

Búsqueda por propiedad o efecto de la sustancia

Investiga bioactividad (efectos, blancos, especies, etc.)

Exporta sustancias y sus datos para planillas y analiza sus relaciones

Campo de Datos
"Isolation from natural product"



Herramienta para planificación de síntesis

The screenshot displays a chemical synthesis planning tool interface. At the top, there are buttons for 'Undo', 'Open', 'Save', and 'Copy plan to new page'. The 'Synthesis representation' is set to 'Left to Right'. The main area shows a reaction scheme with three steps: Step 1 (94.7% yield) converting a starting material to an intermediate, Step 2 (82% yield) converting the intermediate to another intermediate, and Step 3 (82% yield) converting the intermediate to the final product. A red box highlights the 'Synthesize' button for Step 3, with a red arrow pointing to the 'Add' button in the filter panel below. The filter panel includes options for Yield, Record Type, Reagent/Catalyst, Solvent, Reaction Type, and No. of Steps. A table of references is shown below the reaction scheme, listing various publications for each step. A red text box on the right side of the interface contains the text: 'Seleccione la mejor ruta entre diversas publicaciones para optimizar su estrategia de síntesis.'

Step	Yield	Conditions	References
2	94.7%	in CH_2Cl_2	Koul, Surrinder; Koul, Jawahir Lal; Singh, Budh; Kapoor, Munish; Parshad, Rajinder; Manhas, Kuldeep S.; Taneja, Subhash C.; Qazi, Ghulam N. Tetrahedron: Asymmetry, 2005 , vol. 16, # 15 p. 2575 - 2592 Title/Abstract Full Text Scopus
3	82%	With SOCl_2 in toluene T=90°C; 4 h;	Bellucci, Giuseppe; Berti, Giancarlo; Bianchini, Roberto; Vecchiani, Sandra Gazzetta Chimica Italiana, 1988 , vol. 118, # 6 p. 451 - 456 Title/Abstract Full Text
		With thionyl chloride in benzene 3 h; Heating;	Rao, Ch Prasad; Srimannarayana, G; Sundaramurthy, V Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chem Title/Abstract Full Text Scopus
		With SOCl_2 T=90°C; 3 h;	Gualtieri, Fulvio; Conti, Gabriele; Dei, Silvia; Giovannoni, Maria Paola; Nan Journal of Medicinal Chemistry, 1994 , vol. 37, # 11 p. 1704 - 1711 Title/Abstract Full Text Scopus

161 reactions out of 117 citations go to Page 1 of 18

Sort by Reaxys-Ranking

Filter by:
Yield
Record Type
Reagent/Catalyst
Solvent
Reaction Type
No. of Steps

Add

Yield Conditions References
CC(C)C(C)C1=CC=C(C=C1)C(=O)O
Rx-ID: 1062590

Done Internet

Compare estructuras y sus datos

reaxys

Output Substance Results

Output Substance Grid Substance Details Table Substance Citations Table

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

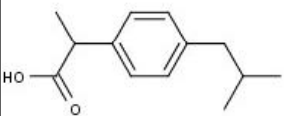
RD File SD/Molfile Smiles

Include the following headline

Output range All Hits Selected hits Range: e.g. 1, 2-5, 10

Output contains include Structures All available data Identification data only Select data

Exporte estructuras y sus datos en XLS, WORD, PDF

Structure	Reaxys RegNo	CAS Registry Number	Pharmacological Data: Effect	Species or Test-System	Method	Further Details	Type	Value of Type	References
	2049713	15687-27-1; 51146-56-6; 51146-57-7; 58560-75-1	enzyme activity; inhibition of	recombinant aldo-keto reductase 1C1	enzyme incubated with title comp.; enzyme activity determined using 9,10-phenanthrene quinone substrate	1C1: 20 α -hydroxysteroid dehydrogenase	IC50	29 μ mol/l	Journal; Byrns, Michael C.; Steckelbroeck, Stephan; Penning, Trevor M.; Biochemical Pharmacology; vol. 75; 2; (2008); p. 484 - 493;

Resumiendo

- Reaxys reduce el tiempo necesario para encontrar resultados relevantes
- Interfaces simples, poderosa herramienta de búsqueda y contenido indexado con foco en la síntesis química
- Extenso repositorio de propiedades químicas y datos experimentales de reacciones
- Información extraída de la literatura científica y de patentes



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