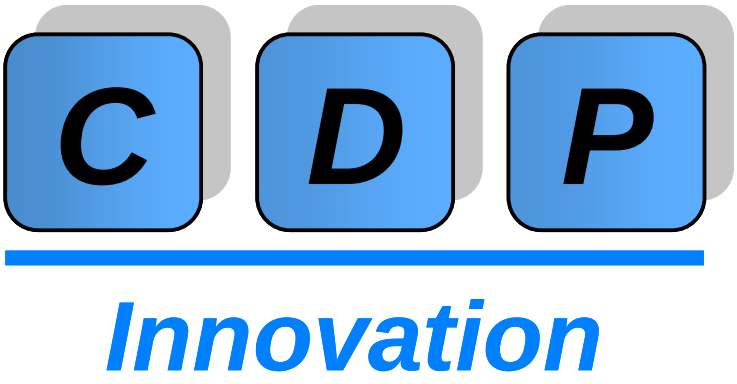

CDP DATA BASES

(Issue January 2019)

CDP-INNOVATION
G2C Business center, 63 Rue André Bollier, 69007 Lyon cedex 07, France
Société par Actions Simplifiées au capital de 39000 €
482 740 503 RCS Lyon

Fragrances and Flavor Data Base (version 4.4) 5720 € HT*

This base describes the molecules used in the fields of perfumery or the aromas with their organoleptic properties. She mentions both commercial products and non-commercial products. For commercial products, a list of suppliers is indicated. Version 4.4 contains 4400 products.

Possible search by:
- structures and sub-structures
- chemical names
- common names
- RN-CAS
- FEMA number
- ECHA number
- EINECS number
- olfactory properties
- organoleptic properties
- limits of detection
- substantivity
- naturalness and occurrence of the product
- physicochemical characteristics
- current industrial suppliers
- previous industrial suppliers
- occurrence

Possibility of Multicriteria research

* Databases are provided as SDF/RDF files recognized by the majority of chemical structure softwares.

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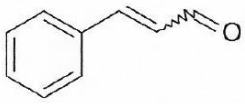
FRAGRANCES AND FLAVORS DATA BASE

ID: 26

CHEMICAL NAME:

3-Phenyl-2-propenal

CHEMICAL STRUCTURE:



NATURAL STRUCTURE:	AVAILABILITY:	FORMULA:	MOLECULAR WEIGHT:
Yes	Commercial	C_9H_8O	132.16

NATURAL OCCURRENCE:

Beer Cassia Celery seed Sour cherry Cinnamon Clove stem
Cognac Guava Lemon balm Black tea Tomato Red wine

CAS NUMBER: 104-55-2-

FEMA NUMBER: 2286

ECHA NUMBER: 100.002.922

EC NUMBER: 203-213-9

FLASH POINT (°C): 71

BOILING POINT (°C): 250

PRESSURE (mmHg): 760.00

CHIRALITY: No

E-Z ISOMERS: Yes

LOG P: 1.900

NAMES:

Aldehyde cnnamique naturel (153)
Cassia aldehyde
Cinnamal
Cinnamaldehyde (44)
Cinnamaldehyde natural (44)
Cinnamic aldehyde (48,145,158)
Cinnamic aldehyde FCC (186)
Cinnamic aldehyde natural (145,158,186)

SUPPLIERS:

Fleurchem (145)
Mane (176)
Prodasynth (153)
SAFC Flavors & Fragrances (44)
Symrise (158)
Vigon (186)

EX SUPPLIERS:

Quest (48)

MELTING POINT (°C):	DENSITY:	ODOR THRESHOLD (ng/l air)	TASTE THRESHOLD (ng/l water)	SUBSTANTIVITY:
-7.5	1.0480			212.0

ODOR:

Sweet spicy, warm, woody cinnamic, cinnamon bark, phnolic clove-like with a fruity resinous nuance (4).
Cinnamon, clove, spicy (44).

TASTE:

Sweet spicy, warm cinnamic, sweet medicinal with a fruityphenolic nuance (4).
Cinnamon, spicy, fragrant, clove, sweet, cassia, burning, aromatic taste (44).

FRAGRANCE APPLICATIONS:

Gives a warm spicy twist. Particularly useful in white florals (48).

FLAVOR APPLICATIONS:

Cinnamon, spicy nuances, cola, spice blends, confections, oral care products and chewing gums (149).

Names of Chemical Reactions (version 0.49) 637 € HT*

The Names of Chemical Reactions database is both a tool of creativity to search for synthetic methods for a product, to find reactions sometimes unknown to the chemist to achieve a transformation and a teaching tool self-study describing the mechanisms. Version 0.49 describes the mechanisms of 490 reactions with their mechanisms.

Possible search by:
- name of reaction
- structure (reactants or products formed or desired transformations)
- reaction intermediates
- conditions
- mechanism

Possibility of Multicriteria research

The base also gives references in which this reaction has been used.

* Databases are provided as SDF/RDF files recognized by the majority of chemical structure softwares.

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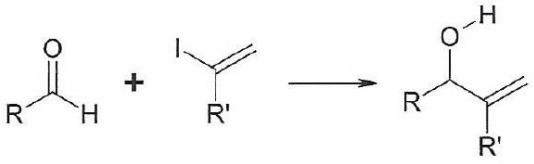
NAMES OF CHEMICAL REACTIONS DATA BASE

ID: 465

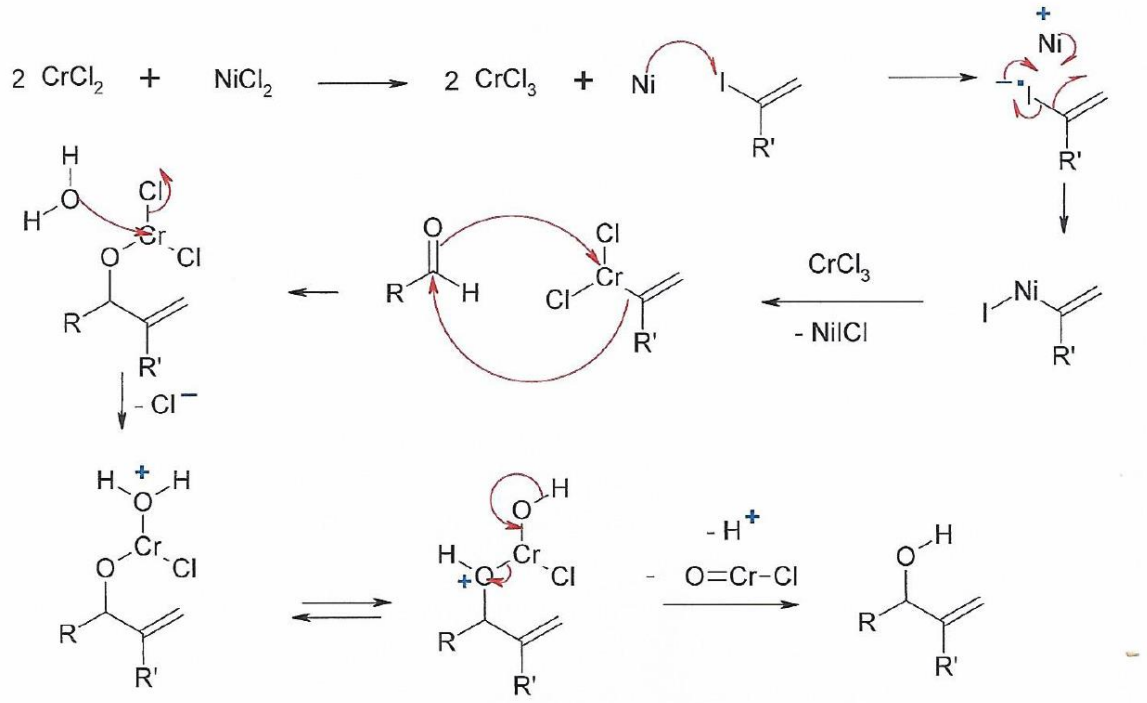
REACTION NAME:

Nozaki-Hiyama-Takai-Kishi reaction

EQUATION:



MECHANISM:



REAGENTS:

Aldehydes
Vinyl iodide

CONDITIONS:

Reagent (CrCl2)
Catalyst (NiCl2)
Solvent (DMF, DMSO,....)

PRODUCTS:

Allylic alcohols

REACTION TYPES:

Coupling
Nozaki-Hiyama-Takai-Kishi

LITERATURE:

1-Role of the Nozaki-Hiyama-Takai-Kishi reaction in the synthesis of natural products, A. Gil, F. Albericio, M. Alvarez*, Chem. Rev., (2017), 117, 8420-8446.

COMMENTS:

Chemical Reactions **(version 1.5)** **750 € HT***

Chemical Reactions is a compilation of original and recent reactions. Reactions in the base also were chosen because of their high yields and their general character. This version contains 1500 recent reactions. This base also is a tool to increase creativity.

Possible search by:
- substructures
- reaction
- reagents
- structure of ligands
- authors
- university or company

.....

Possibility of Multicriteria research

* Databases are provided as SDF/RDF files recognized by the majority of chemical structure softwares.

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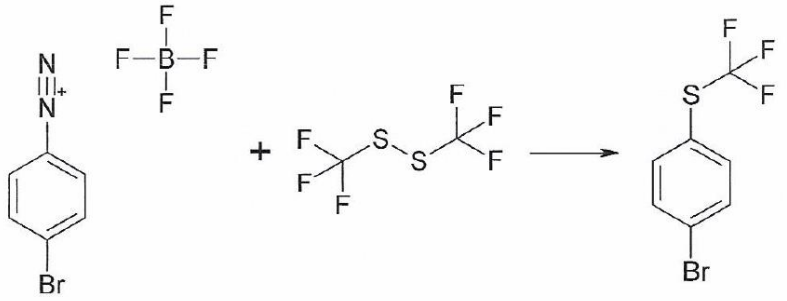
CHEMICAL REACTIONS DATA BASE

ID: 1469

TITLE:

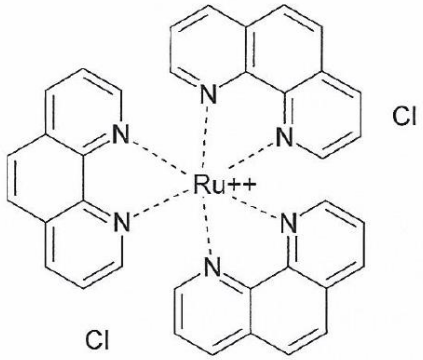
Radical aromatic trifluoromethylthiolation: photoredox catalysis vs. base mediation

REACTION:



CONDITIONS:	REACTION SOLVENT:	REACTION TEMPERATURE (°C):
t=1h 1 Eq. of F3SSCF3 0.5 mol% of [Ru(bpy)3]Cl2 LED (450nm)	Dimethysulfoxide	20

CATALYST OR LIGAND:



YIELD (%): 58.0

CONVERSION (%):

SELECTIVITY (%):

ASYMMETRIC REACTION: No

STEREOSELECTIVITY:

COMPOUND:

COMPOUND:

TRANSFORMATION: Chemical

REACTION NAMES: Trifluoroythiomethylation

STRAINS OR ENZYMES OR PLANTS:

ELEMENT: Ruthenium

AUTHORS:

D. Koziakov, M. Majek, A. Jacobi von Wangelin*

REVIEW:

Eur. J. Org. Chem., (2017), 6722-6725

ADDRESS

Institute of Organic Chemistry, University of Regensburg, Germany
Department of Chemistry, University of Hamburg, Martin Luther King Platz 6, 20146 Hamburg, Germany

PATENT NUMBER:	APPLICATION DATE:	COMPANY:

Cosmetics Data Base (version 1.8) 2700 € HT*

This base describes the molecules used in the areas of cosmetics with their physical-chemical properties and the claimed properties. It mentions mainly commercial products. For commercial products, a list of suppliers is indicated. Version 1.8 contains 1800 products.

Possible by search
- structures and substructures
- chemical names
- common names
- INCI name
- RN-CAS
- FEMA number
- ECHA number
- EINECS number
- China number
- INCI properties
- cosmetic properties
- odor
- solubility
- toxicological and ecotoxicological data.
- naturalness and occurrence of the product
- physicochemical characteristics including Log P
- current industrial suppliers
- previous industrial suppliers

Possibility of Multicriteria research

* Databases are provided as SDF/RDF files recognized by the majority of chemical structure softwares.

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COSMETICS DATA BASE

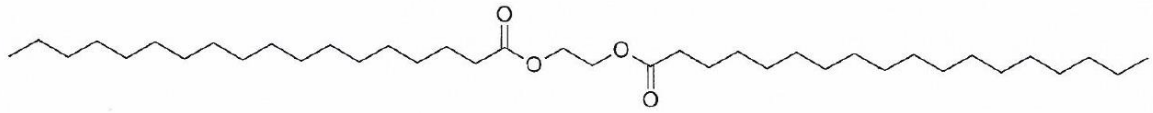
ID: 33

CHEMICAL NAME: 1,2-Ethanediyl bis(octadecanoate)

INCI NAME: GLYCOL DISTEARATE

INCI CLASS: Emollient

CHEMICAL STRUCTURE:



NATURAL STRUCTURE:	AVAILABILITY:	FORMULA:	MOLECULAR WEIGHT:
No	Commercial	$C_{38}H_{74}O_4$	595.01

NATURAL OCCURRENCE:

CAS NUMBER: 627-83-8

FEMA:

NAMES:
Alkalmuls 504/V (45)
Cithrol EGDS (9)
1,2-Ethanediyl bis(octadecanoate)
Ethylene distearate
Glycerol stearate

ECHA NUMBER: 100.010.014

EC NUMBER: 211-014-3

COSMETICAL SPECIALITIES:
Mackadet BWC-CL {cocamide MEA, cocamidopropyl betaine, disodium oleamido MEA-sulfosuccinate, glycol distearate, propylene glycol, sodium laureth sulfate, sodium lauryl sulfate} (45)
Saboperl 500 {cocamide MEA, glycol distearate, laureth-10, sodium laureth

CHINA NUMBER: 5627

FLASH POINT (°C):

BOILING POINT (°C):

SUPPLIERS:
HallStar (3)
Croda (9)
Sabo (39)
Solvay (45)

EX SUPPLIERS:

PRESSURE (mmHg):

CHIRALITY:	E-Z ISOMERS:
No	No

MELTING POINT (°C):	DENSITY:	ABSORPTION:	RI:	LOG P:	TOXICITY-ECOTOXICITY:
62.0				16.120	Toxicological information: Acute oral toxicity LD50 (rat): dose

ODOR:

PROPERTIES:
Bodying agent (3).
Emollient (45).

USES:
Facial cleansers, foot care, hair colorants, hair conditioners, liquid handsoaps, shampoos, shower gels, styling aids (3).

SOLUBILITY:
Ethanol hot [9003-99-0]: soluble
Isopropanol hot [67-63-0]: soluble

MINIMUM INHIBITORY CONCENTRATION (PPM):

Pharma Data Base (version 0.7) 1400 € HT*

This base describes the molecules used in the fields of pharma with their physical, chemical and pharmacological properties. It mentions mainly active ingredients, but also of nutraceuticals, or excipients. Version 0.7 includes 700 products. All new products recently approved by the FDA are systematically recorded.

Possible research by:
- structures or substructures
- disease area
- by class of includes (active ingredients, excipients, biologics,..)
- chemical names
- common names
- trade names
- RN-CAS
- ECHA number
- EINECS number
- pharmacological properties
- toxicological and ecotoxicological data
- naturalness and occurrence of the product
- physicochemical characteristics including Log P
- current industrial suppliers
- previous industrial suppliers
- originator or generic products with expiry date of patent

Possibility of multicriteria research

* Databases are provided as SDF/RDF files recognized by the majority of chemical structure softwares.

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PHARMA DATA BASE

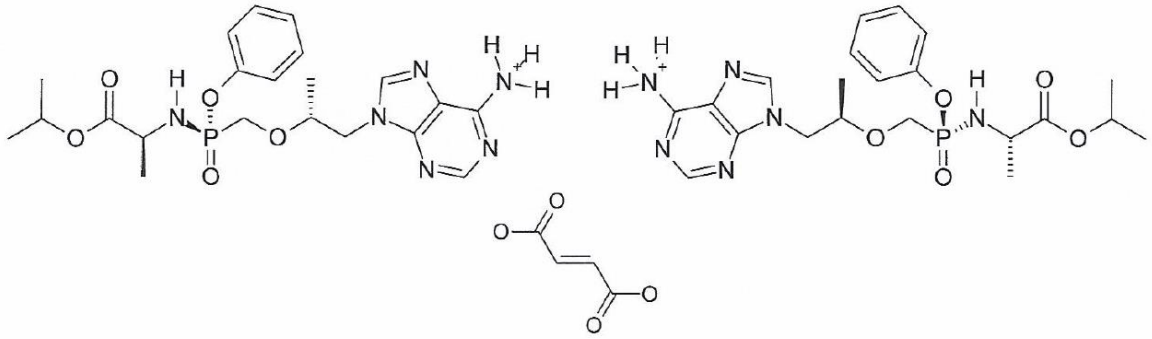
ID: 503

CHEMICAL NAME: Bis(propan-2-yl (2S)-2-[[[(2R)-1-(6-aminopurin-9-yl)propan-2-yl]oxymethyl-phenoxyphosphoryl]amino]propanoate) (E)-but-2-enedioate

THERAPEUTIC USES: Virology (Hepatitis B)

CATEGORY: Active ingredients

CHEMICAL STRUCTURE:



NATURAL STRUCTURE: No

AVAILABILITY: Commercial
See tenofovir alafenamide

FORMULA: $C_{46}H_{62}N_{12}O_{14}P_2$

MOLECULAR WEIGHT: 1069.03

NATURAL OCCURRENCE:

APPROVAL DATE:
EU 19/11/2015
EU 21/06/2016

CAS NUMBER: 1392275-56-7

ATC CLASSIFICATION: J05AF13

DCI AND OTHER NAMES: Bis(propan-2-yl (2S)-2-[[[(2R)-1-(6-aminopurin-9-yl)propan-2-yl]oxymethyl-phenoxyphosphoryl]amino]propanoate) (E)-but-2-enedioic acid
Bis(propan-2-yl (2S)-2-[[[(2R)-1-(6-aminopurin-9-yl)propan-2-yl]oxymethyl-phenoxyphosphoryl]a

ECHA NUMBER:

EC NUMBER:

BRAND NAME: Biktarvy
Descovy
Genvoya
Odefsey
Vemlidy

PHARMACEUTICAL LABORATORIES:
France
Gilead
USA

FLASH POINT (°C):

BOILING POINT (°C):

PRESSURE (mmHg):

API SUPPLIERS:

API EX-SUPPLIERS:

CHIRALITY: Yes

E-Z ISOMERS: Yes

MELTING POINT (°C):	DENSITY:	ABSORPTION:	RI:	LOG P:	TOXICITY-ECOTOXICITY:

POSOLOGY:
Adult: 25 mg/day

DOSAGE FORM:
Tablets

PROPERTIES-USES:
Nucleotide reverse transcriptase inhibitor

COMMENTS:
EU 19/11/2015: EMA approved Genvoya.
EU 21/06/2016: EMA approved Odefsey.

SOLUBILITY:

ORIGINATOR & APPLICATION DATE:
Gilead
WO 2013025788 A1 (16/08/2011)

STATUS:
Princeps (2031)

Parapharmaceutical Data Base (version 0.1) 200 € HT*

This base describes the molecules used in the areas of the drugstore with their physicochemical properties and the claimed properties. It mentions mainly commercial products. For commercial products, a list of suppliers is mentioned. The version 0.1 contains 100 products.

Possible search by:
- structures and substructures
- chemical names
- common names
- parapharmaceutical specialties
- application areas
- laboratories marketing parapharmaceutical specialties
- RN-CAS
- FEMA number
- ECHA number
- EINECS number
- properties
- solubility
- toxicological and ecotoxicological data.
- naturalness and occurrence of the product
- physicochemical characteristics including Log P
- current industrial suppliers
- previous industrial suppliers

Possibility of Multicriteria research

* Databases are provided as SDF/RDF files recognized by the majority of chemical structure softwares.

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PARAPHARMACEUTICAL DATA BASE

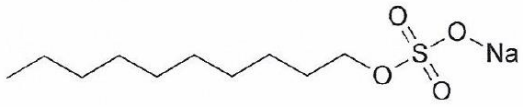
ID: 8

CHEMICAL NAME: Sodium monododecyl sulfate

USES: Dermatology

FUNCTIONS: Formulation (Surfactant)

CHEMICAL STRUCTURE:



NATURAL STRUCTURE:	AVAILABILITY:	FORMULA:	MOLECULAR WEIGHT:
No	Commercial	$C_{10}H_{21}NaO_4S$	260.33

NATURAL OCCURRENCE:

CAS NUMBER: 151-21-3

OTHER NAMES:
Naterol N70
Naterol N95
Naterol P90-USP
Sabosol LSS/P
Sodium lauryl sulfate
Sodium lauryl sulphate

FEMA NUMBER:

ECHA NUMBER: 100.005.263

EC NUMBER: 205-788-1

PARAPHARMACEUTICAL SPECIALITIES INGREDIENTS:
Addax mains Hycalaia 75 {allantoin, aqua, bisabolol, butylphenyl methylpropional, butyrospermum parkii, C13-14 isoparaffin, cinnamic alcohol, citronellol, cetearyl alcohol, citric acid, coco-caprylate/caprate, coumarin, dimethiconol, geraniol, glycerin, hexyl cinnamal, imidazolidinyl urea, alpha-isomethyl ionone, laureth-7, limonene, linalool, methylparaben, parfum, polyacrylamide, propylparaben, retinyl palmitate, sodium cetearyl sulfate,

FLASH POINT (°C):

BOILING POINT (°C):

PRESSURE (mmHg):

CHIRALITY: No

E-Z ISOMERS: No

PHARMACEUTICAL LABORATORIES:	INGREDIENT SUPPLIERS:
France Omega Pharma (1)	Croda Cisme

MELTING POINT (°C):	DENSITY:	ABSORPTION:	RI:	LOG P:	TOXICITY-ECOTOXICITY:

POSOLOGY:

DOSAGE FORM: Cream

PROPERTIES-USES:
Emulsifier
Foaming

COMMENTS:
Addax mains Hycalia 75: moisturizer and anti-roughness cream (1).

SOLUBILITY:	ORIGINATOR & APPLICATION DATE:	STATUS:
	Standard Oil Development US 2393152 (16/07/1940)	Generic

Do not hesitate to ask for a demonstration to the representative of CDP-Innovation during training

Information from info@cdp-innovation.com

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