

CASTELLANOS & CO LTDA
ABOGADOS
Calle 94 A No.7ª-09
Bogotá D.C. - Colombia

SUPERINTENDENCIA DE INDUSTRIA Y COMERCIO



No. 09-135635- -00005-0000

Fecha: 2012-11-02 14:41:51 Dep. 2020 DIR.NUEVASOR
Tra. 11 PATENTEIYII Eve: 378 FASENACIONALI
Act. 523 RESPUESTA Folios: 20

Señor Director

División de Nuevas Creaciones

Superintendencia de Industria y Comercio
Ministerio de Comercio, Industria y Turismo

E. S. D.

Re.: Expediente No. 09 135635

Solicitud de Patente de invención para: "PROCESO PARA LA PRODUCCIÓN DE
PIRAZOLES"

Solicitante: SYNGENTA LIMITED - SYNGENTA PARTICIPATIONS AG

RESPUESTA AL EXAMEN DE BUSQUEDA DE
ANTERIORIDADES

MARGARITA CASTELLANOS ABONDANO, mayor de edad, identificada y domiciliada como aparece al pie de mi firma, en atención a su oficio No. 14140 notificado el 14 de Agosto de 2012, atentamente me permito dar repuesta al mismo de la siguiente manera:

Presento copia completa de los artículos requeridos por ese Despacho como resultado de la búsqueda de anterioridades:

- DATABASE CASREACT CHEMICAL ABSTRACTS SERVICE, COLUMBUS, OHIO, US; XP002454520 retrieved from STN Database accession no. 145: 271773 - & WO2006/090778 A (SAGAMI CHEMICAL RESEARCH CENTER)

31 August 2006 (2006-08-31).

- DATABASE CAPLUS CHEMICAL ABSTRACTS SERVICE, COLUMBUS, OHIO, US; XP002455007 retrieved from STN Database accession no. 2002:344916- & JP 2002 128763 A (MITSUI CHEMICALS INC) 9 May 2002 (2002-05-09).
- "CRC HANDBOOK OF CHEMISTRY AND PHYSICS, 76th Edition" 1995, CRC PRESS, BOCA RATON, US, XP002455005 page 3-1; page 3-144, compound no. 5187; page 3-246, compound no. 8981.

Cumplido así con lo dispuesto, atentamente solicito a Ud. se continúe con el trámite correspondiente a esta solicitud de Patente de Invención.

Del Señor Director,


Margarita Castellanos Abondano

C.C. No. 39.779.654 de Usaquén

T.P.A. No.70819 del C. Sup. de la Judicatura.

Calle 94 A No.7A-09 – Bogotá D.C.

Teléfonos: 7560770 y 7550158

Bogotá, D.C.

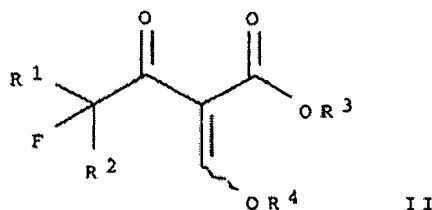
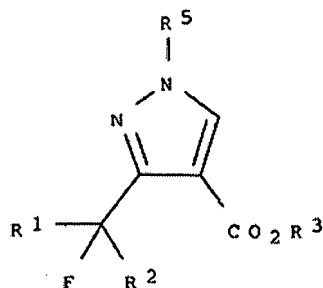
02 NOV. 2012

XP-002454520

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L1 ANSWER 1 OF 1 CASREACT COPYRIGHT 2007 ACS on STN
 AN ***145:271773*** CASREACT
 TI Method for producing alkyl 1-alkyl-3-fluoroalkyl pyrazole-4-carboxylate
 IN Aihara, Hidenori; Yokota, Wakako; Yamakawa, Tetsu; Hirai, Kenji
 PA Sagami Chemical Research Center, Japan
 SO PCT Int. Appl., 32pp.
 CODEN: PIXXD2
 DT Patent
 LA Japanese
 CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006090778	A1	20060831	WO 2006-JP303269	20060223
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM IN 2007DN06200 A 20070831 IN 2007-DN6200 20070809 PRAI JP 2005-52004 20050225 JP 2005-52006 20050225 WO 2006-JP303269 20060223 OS MARPAT 145:271773 GI				



AB There is disclosed a method for producing alkyl 1-alkyl-3-fluoroalkyl pyrazole-4-carboxylate [I; R1 = H, halo; R2 = H, F, Cl, F, Cl-12 alkyl optionally substituted by F atom; R3 = Cl-6 alkyl; R5 = (un)substituted Cl-6 alkyl] by cyclocondensation of alkyl 2-alkoxymethylenefluoroacetylacetate (II; R1-R3 = same as above; R4 = Cl-6 alkyl) and a alkylhydrazine of formula R5NHNH2 [R5 = (un)substituted Cl-6 alkyl]. By performing the reaction in the presence of a base and water, 1-alkyl-3-fluoroalkyl pyrazole-4-carboxylate I can be highly selectively produced with high

yield. This novel method enables to highly selectively produce 1-alkyl-3-fluoroalkyl pyrazole-4- carboxylate I, which is useful as an intermediate for pharmaceutical and agrochem. products, with high yield by simple and safe operations. Thus, 0.097 mL 2-ethoxymethylene-4,4,4-trifluoroacetoacetic acid Et ester was added dropwise to a mixt. of a soln. of 20 mg NaOH in 5.0 mL H₂O and 0.197 mL 35 wt.% methylhydrazine soln. with stirring under ice-cooling and the resulting mixt. was stirred at the same temp. for 1 h and neutralized by adding 1 N aq. HCl soln. to give, after workup, a 98:2 mixt. of 1-methyl-3-trifluoromethylpyrazole-4-carboxylic acid Et ester (III) and 1-methyl-5-trifluoromethylpyrazole-4-carboxylic acid Et ester (IV) in 86% yield. When the same reaction was carried out without the base, a 66:34 mixt. of III and IV was obtained in 91% yield.

- ST sodium hydroxide potassium hydroxide cyclocondensation catalyst; alkyl alkylfluoroalkylpyrazolecarboxylate prepn; cyclocondensation alkyl alkoxymethylenefluoroacylacetate alkyl alkylhydrazine
- IT Regiochemistry
(prepn. of alkyl 1-alkyl-3-fluoroalkylpyrazole-4-carboxylate by regioselective cyclocondensation of alkyl 2-alkoxymethylenefluoroacylacetate with alkylhydrazine in presence of sodium or potassium hydroxide)
- IT Cyclocondensation reaction
Cyclocondensation reaction catalysts
(regioselective; prepn. of alkyl 1-alkyl-3-fluoroalkylpyrazole-4-carboxylate by regioselective cyclocondensation of alkyl 2-alkoxymethylenefluoroacylacetate with alkylhydrazine in presence of sodium or potassium hydroxide)
- IT 7732-18-5, Water, uses
RL: NUU (Other use, unclassified); USES (Uses)
(prepn. of alkyl 1-alkyl-3-fluoroalkylpyrazole-4-carboxylate by regioselective cyclocondensation of alkyl 2-alkoxymethylenefluoroacylacetate with alkylhydrazine in presence of sodium or potassium hydroxide)
- IT 111493-74-4P, 1-Methyl-3-trifluoromethylpyrazole-4-carboxylic acid ethyl ester 231285-86-2P, 1-Methyl-5-trifluoromethylpyrazole-4-carboxylic acid ethyl ester
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of alkyl 1-alkyl-3-fluoroalkylpyrazole-4-carboxylate by regioselective cyclocondensation of alkyl 2-alkoxymethylenefluoroacylacetate with alkylhydrazine in presence of sodium or potassium hydroxide)
- IT 60-34-4, Methylhydrazine 571-55-1, 2-Ethoxymethylene-4,4,4-trifluoroacetoacetic acid ethyl ester 624-80-6, Ethylhydrazine 5039-61-2, Propylhydrazine 42504-87-0, Isobutylhydrazine 176969-33-8, 2-Ethoxymethylene-4,4-difluoroacetoacetic acid ethyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(prepn. of alkyl 1-alkyl-3-fluoroalkylpyrazole-4-carboxylate by regioselective cyclocondensation of alkyl 2-alkoxymethylenefluoroacylacetate with alkylhydrazine in presence of sodium or potassium hydroxide)

IT 1310-58-3, Potassium hydroxide, reactions 1310-73-2, Sodium hydroxide, reactions

RL: RGT (Reagent); RACT (Reactant or reagent)

(prepn. of alkyl 1-alkyl-3-fluoroalkylpyrazole-4-carboxylate by regioselective cyclocondensation of alkyl 2-alkoxymethylene fluoroacylacetate with alkylhydrazine in presence of sodium or potassium hydroxide)

IT 141573-95-7P, 1-Methyl-3-(difluoromethyl)pyrazole-4-carboxylic acid ethyl ester 155377-12-1P, 1-Ethyl-3-(trifluoromethyl)pyrazole-4-carboxylic acid ethyl ester 851725-98-9P, 1-Methyl-5-(difluoromethyl)pyrazole-4-carboxylic acid ethyl ester 907199-71-7P, 1-Ethyl-5-(trifluoromethyl)pyrazole-4-carboxylic acid ethyl ester 907199-72-8P, 1-Propyl-3-(trifluoromethyl)pyrazole-4-carboxylic acid ethyl ester 907199-73-9P, 1-Propyl-5-(trifluoromethyl)pyrazole-4-carboxylic acid ethyl ester 907199-74-0P, 1-Isobutyl-3-(trifluoromethyl)pyrazole-4-carboxylic acid ethyl ester 907199-75-1P, 1-Isobutyl-5-(trifluoromethyl)pyrazole-4-carboxylic acid ethyl ester

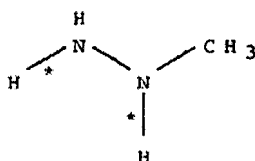
RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of alkyl 1-alkyl-3-fluoroalkylpyrazole-4-carboxylate by regioselective cyclocondensation of alkyl 2-alkoxymethylene fluoroacylacetate with alkylhydrazine in presence of sodium or potassium hydroxide)

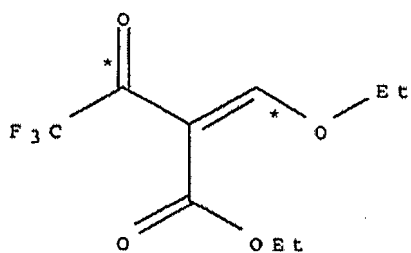
RE.CNT 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE

- (1) Basf Aktiengesellschaft; WO 2005123690 A1 2005 CAPLUS
- (2) Mitsui Chemicals Inc; EP 1067121 A2 2001 CAPLUS
- (3) Mitsui Chemicals Inc; JP 200158982 A 2001
- (4) Mitsui Chemicals Inc; US 6235911 B1 2001 CAPLUS
- (5) Nippon Hydrazine Kogyo Kabushiki Kaisha; JP 08-269014 A 1996 CAPLUS
- (6) Sankyo Aguro Kabushiki Kaisha; EP 1580189 A1 2004 CAPLUS
- (7) Sankyo Aguro Kabushiki Kaisha; CN 1732155 A 2004 CAPLUS
- (8) Sankyo Aguro Kabushiki Kaisha; WO 2004060877 A1 2004 CAPLUS
- (9) Ube Industries Ltd; JP 10-175957 A 1998 CAPLUS
- (10) Ube Industries Ltd; US 5808092 A 1998 CAPLUS
- (11) Ube Industries Ltd; EP 837058 A1 1998 CAPLUS

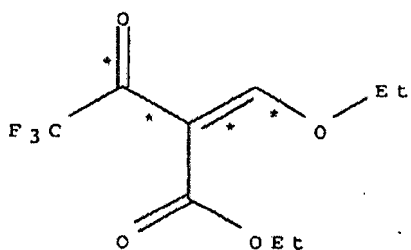
RX(1) OF 5 2 A + 2 B ==> C + D



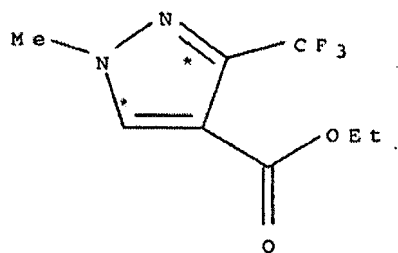
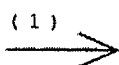
2 A



B

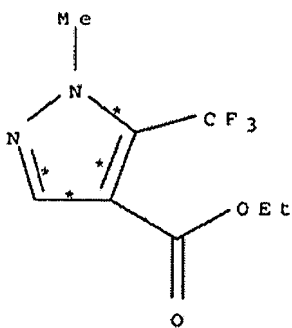


B



C

YIELD 81% (93)



D

YIELD 81% (7)

RX(1) RCT A 60-34-4, B 571-55-1

STAGE(1)

RGT E 1310-58-3 KOH

SOL 7732-18-5 Water

CON SUBSTAGE(1) room temperature -> 0 deg C

SUBSTAGE(2) 1 hour, 0 deg C

STAGE(2)

RGT F 7647-01-0 HCl

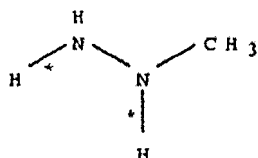
SOL 7732-18-5 Water

CON neutralized

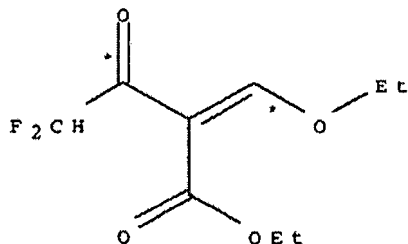
PRO C 111493-74-4, D 231285-86-2

NTE alternative prepn. shown

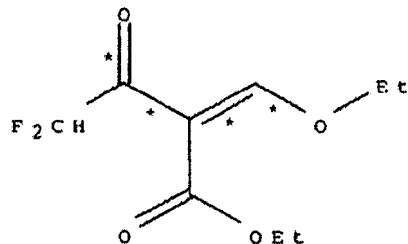
---(2) OF 5 2 A + 2 H ==> I + J



2 A

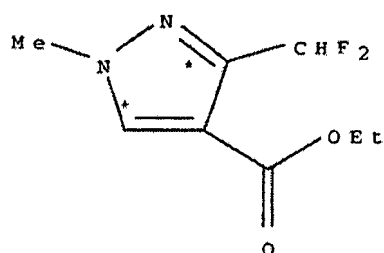


H



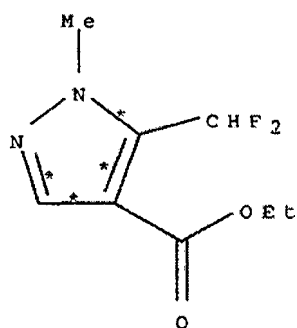
H

(2) →



I

YIELD 86% (94)



J

YIELD 86% (6)

RX(2) RCT A 60-34-4, H 176969-33-8

STAGE(1)

RGT E 1310-58-3 KOH

SOL 7732-18-5 Water

CON SUBSTAGE(1) room temperature -> 0 deg C

SUBSTAGE(2) 1 hour, 0 deg C

STAGE(2)

RGT F 7647-01-0 HCl

SOL 7732-18-5 Water

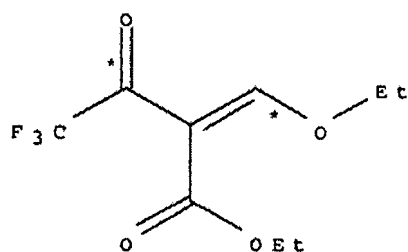
CON neutralized

PRO I 141573-95-7, J 851725-98-9

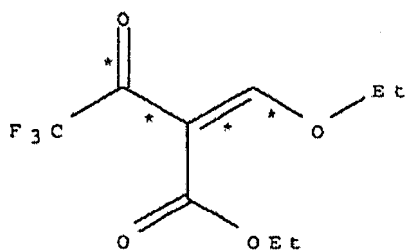
NTE alternative prepn. shown

RX(3) OF 5 2 B + 2 K ==> L + M

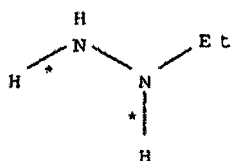
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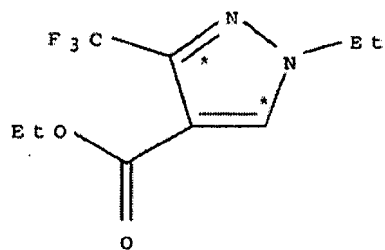
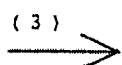
B



B

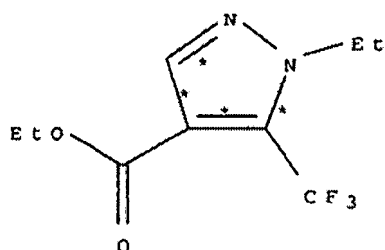


2 K



L

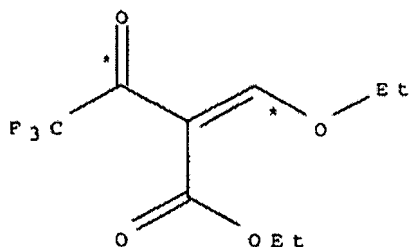
YIELD 89% (89)



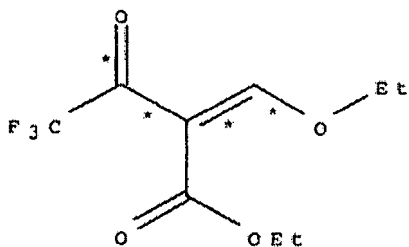
M
YIELD 89% (11)

RX(3) RCT B 571-55-1, K 624-80-6
RGT N 1310-73-2 NaOH
PRO L 155377-12-1, M 907199-71-7
SOL 7732-18-5 Water
CON SUBSTAGE(1) room temperature -> 0 deg C
SUBSTAGE(2) 15 minutes, 0 deg C
SUBSTAGE(3) 10 minutes, 0 deg C
NTE alternative prepn. shown

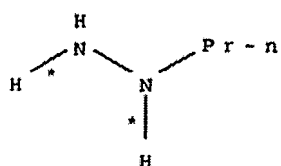
RX(4) OF 5 2 B + 2 O ==> P + Q



B

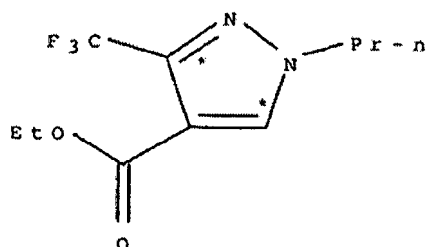


B



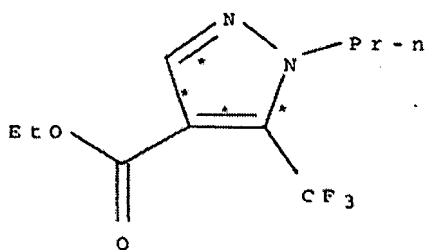
2 0

(4)



P

YIELD 98% (86)

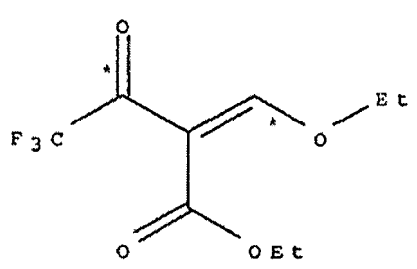


Q

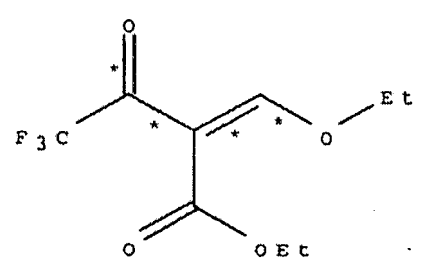
YIELD 98% (14)

RX(4) RCT B 571-55-1, O 5039-61-2
 RGT N 1310-73-2 NaOH
 PRO P 907199-72-8, Q 907199-73-9
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) room temperature -> 0 deg C
 SUBSTAGE(2) 5 minutes, 0 deg C
 SUBSTAGE(3) 10 minutes, 0 deg C
 NTE alternative prepn. shown

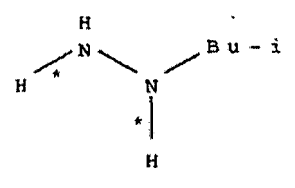
RX(5) OF 5 2 B + 2 R ==> S + T



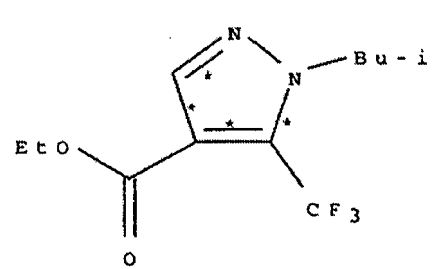
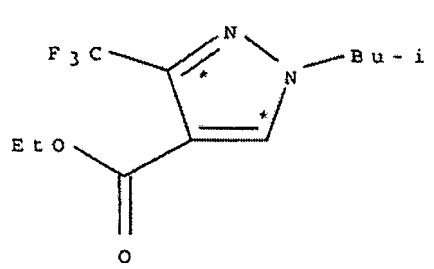
B



B



2 R



S

YIELD 96% (77)

T

YIELD 96% (23)

(5)

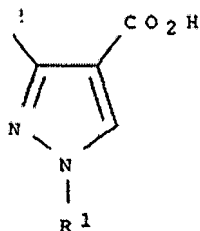
RX(5) RCT B 571-55-1, R 42504-87-0
 RGT N 1310-73-2 NaOH
 PRO S 907199-74-0, T 907199-75-1
 SOL 7732-18-5 Water
 CON SUBSTAGE(1) room temperature--> 0 deg C
 SUBSTAGE(2) 10 minutes, 0 deg C
 NTE alternative prepn. shown

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XP-002455007

LS ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
AN ***2002:344916*** CAPLUS
DN 136:355234
TI Method for purification of 1,3-dialkylpyrazole-4-carboxylic acids
IN Enomoto, Tsuyoshi; Sato, Kenichi
PA Mitsui Chemicals Inc., Japan
SO Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2002128763	A	20020509	JP 2000-328203	20001027
PRAI	JP 2000-328203		20001027		
OS	MARPAT 136:355234				
GI					



AB The title method comprises crystg. a mixt. contg. the title compds. I [R₁ = alkyl; R₂ = H, haloalkyl, etc.] and 1,5-dialkylpyrazole-4-carboxylic acid from an aq. soln. at pH 1.5 to 4.5. The title compds. are pharmaceutical and agrochem. intermediates. Thus, crude 1-methyl-3-trifluoromethylpyrazole-4-carboxylic acid (II) contg. 10.5% 1-methyl-5-trifluoromethylpyrazole-4-carboxylic acid (III) was dissolved in an. aq. soln. of NaOH; HCl was added to the resulting soln. to adjust the pH of the soln. to 3: crystn. was allowed to proceed for 1 h at 20.degree. to give II (contg. 0.6% III) in 95.7% yield.

S. dialkylpyrazolecarboxylic acid purifn pharmaceutical agrochem intermediate; methyltrifluoromethylpyrazolecarboxylic acid purifn pharmaceutical agrochem intermediate

IT Purification
(method for purifn. of 1,3-dialkylpyrazole-4-carboxylic acids)

IT Crystallization
(method for purifn. of 1,3-dialkylpyrazole-4-carboxylic acids by crystn.)

IT ***231285-86-2P***
RL: BYP (Byproduct); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(method for purifn. of 1,3-dialkylpyrazole-4-carboxylic acids)

IT ***113100-53-1P***, 1-Methyl-3-trifluoromethylpyrazole-4-carboxylic acid
RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)

15

(method for purifn. of 1,3-dialkylpyrazole-4-carboxylic acids)

IT ***60-34-4*** , Monomethylhydrazine ***571-55-1*** ,
 2-Ethoxymethylene-3-oxo-4,4,4-trifluorobutyric acid ethyl ester
 RL: RCT (Reactant); RACT (Reactant or reagent)

(method for purifn. of 1,3-dialkylpyrazole-4-carboxylic acids)

IT ***111493-74-4P*** , 1-Methyl-3-trifluoromethylpyrazole-4-carboxylic acid
 ethyl ester
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(method for purifn. of 1,3-dialkylpyrazole-4-carboxylic acids)

IT ***119083-00-0P***
 RL: REM (Removal or disposal); SPN (Synthetic preparation); PREP
 (Preparation); PROC (Process)

(method for purifn. of 1,3-dialkylpyrazole-4-carboxylic acids)

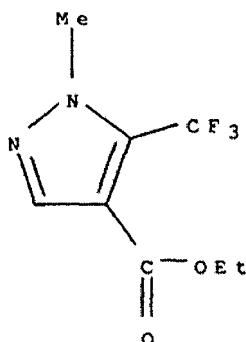
IT ***7732-18-5*** , Water, uses
 RL: NUU (Other use, unclassified); USES (Uses)
 (solvent; method for purifn. of 1,3-dialkylpyrazole-4-carboxylic acids
 by crystn.)

IT ***231285-86-2P***
 RL: BYP (Byproduct); RCT (Reactant); PREP (Preparation); RACT (Reactant or
 reagent)

(method for purifn. of 1,3-dialkylpyrazole-4-carboxylic acids)

RN 231285-86-2 CAPLUS

CN 1H-Pyrazole-4-carboxylic acid, 1-methyl-5-(trifluoromethyl)-, ethyl ester
 (9CI) (CA INDEX NAME)

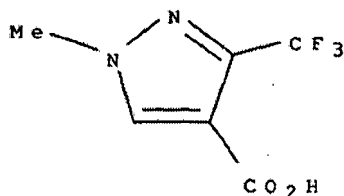


IT ***113100-53-1P*** , 1-Methyl-3-trifluoromethylpyrazole-4-carboxylic acid
 RL: IMF (Industrial manufacture); PUR (Purification or recovery); SPN
 (Synthetic preparation); PREP (Preparation)

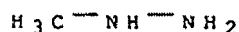
(method for purifn. of 1,3-dialkylpyrazole-4-carboxylic acids)

RN 113100-53-1 CAPLUS

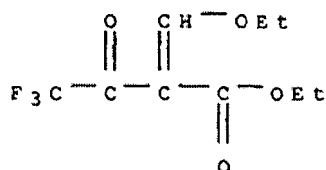
CN 1H-Pyrazole-4-carboxylic acid, 1-methyl-3-(trifluoromethyl)- (CA INDEX
 NAME)



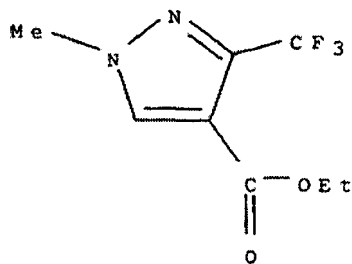
IT ***60-34-4*** , Monomethylhydrazine ***571-55-1*** ,
 2-Ethoxymethylene-3-oxo-4,4,4-trifluorobutyric acid ethyl ester
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (method for purifn. of 1,3-dialkylpyrazole-4-carboxylic acids)
 RN 60-34-4 CAPLUS
 CN Hydrazine, methyl- (CA INDEX NAME)



RN 571-55-1 CAPLUS
 CN Butanoic acid, 2-(ethoxymethylene)-4,4,4-trifluoro-3-oxo-, ethyl ester
 (9CI) (CA INDEX NAME)

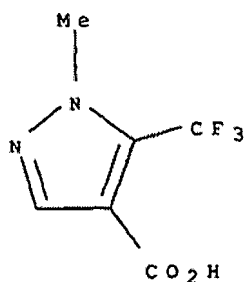


IT ***111493-74-4p*** , 1-Methyl-3-trifluoromethylpyrazole-4-carboxylic acid
 ethyl ester
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (method for purifn. of 1,3-dialkylpyrazole-4-carboxylic acids)
 RN 111493-74-4 CAPLUS
 CN 1H-Pyrazole-4-carboxylic acid, 1-methyl-3-(trifluoromethyl)-, ethyl ester
 (CA INDEX NAME)



IT ***119083-00-0p***
 RL: REM (Removal or disposal); SPN (Synthetic preparation); PREP
 (Preparation); PROC (Process)
 (method for purifn. of 1,3-dialkylpyrazole-4-carboxylic acids)
 RN 119083-00-0 CAPLUS
 CN 1H-Pyrazole-4-carboxylic acid, 1-methyl-5-(trifluoromethyl)- (9CI) (CA

INDEX NAME)



IT ***7732-18-5*** , Water, uses

RL: NUU (Other use, unclassified); USES (Uses)

(solvent; method for purifn. of 1,3-dialkylpyrazole-4-carboxylic acids
by crystn.)

RN 7732-18-5 CAPLOS

CN Water (CA INDEX NAME)

H₂O

=>

EUROPEAN PATENT OFFICE

Patent Abstracts of Japan

PUBLICATION NUMBER : 2002128763
PUBLICATION DATE : 09-05-02

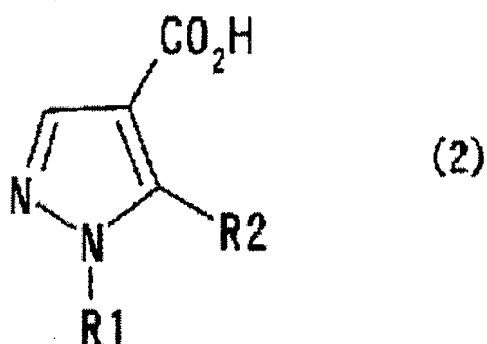
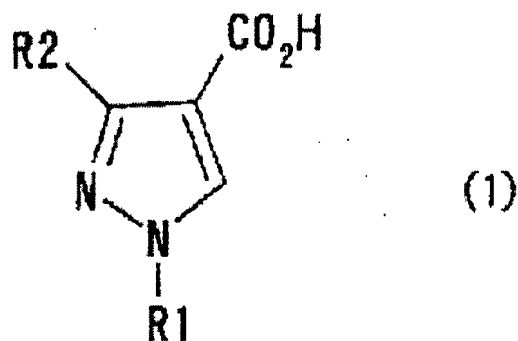
APPLICATION DATE : 27-10-00
APPLICATION NUMBER : 2000328203

APPLICANT : MITSUI CHEMICALS INC;

INVENTOR : SATO KENICHI;

INT.CL. : C07D231/14

TITLE : METHOD FOR PURIFYING
1,3-DIALKYLPIRAZOLE-4-CARBOXYLIC
ACID



ABSTRACT : PROBLEM TO BE SOLVED: To provide a method for isolating and purifying a 1,3-dialkylpyrazole-4- carboxylic acid from the isomer, a 1,5-dialkylpyrazole-4-carboxylic acid.

SOLUTION: This method for isolating the 1,3-dialkylpyrazole-4-carboxylic acid is characterized by regulating an aqueous solution containing the 1,3-dialkylpyrazole-4-carboxylic acid represented by general formula (1) (wherein, R1 denotes a 1-10C chain or cyclic alkyl group; R2 denotes hydrogen atom, a halogen atom, a 1-10C alkyl group or a haloalkyl group) and the 1,5- dialkylpyrazole-4-carboxylic acid represented by general formula (2) (wherein, R1 and R2 denote each the same meaning as that described above) to pH 1.5-4.5 and crystallizing the 1,3-dialkylpyrazole-4-carboxylic acid.

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XP-002455005

PHYSICAL CONSTANTS OF ORGANIC COMPOUNDS (continued)

No.	Name Synonym	Mol. Form. Mol. Wt.	CAS RN mp°C	Merck No. bp°C	Boil. Ref. dens g cm ⁻³	Solubility n _D
5169	Dicarbolic acid, diethyl ester Pyrocarbonic acid diethyl ester	C ₈ H ₁₀ O ₅ 162.14	1609-47-6	8008 83-4 ¹⁸	4-03-00-00018 1.120 ²⁰	ace 4; EtOH 4; lig 4 1.366 ²⁰
5170	Dichlorvos Phosphoric acid, 2,2-dichloroethyl dimethyl ester	C ₄ H ₇ Cl ₂ O ₄ P 220.88	62-73-7	3089 140 ²⁰ ; 64 ¹	1.415 ²⁵	
5171	Dichlorop-methyl Propanoic acid, 2-[4-(2,4-dichlorophenoxy)phenyl]-, methyl ester	C ₁₈ H ₁₄ Cl ₂ O ₄ 341.19	51338-27-3 40	3072 176 ^{0.1}		
5172	Dicrotophos Phosphoric acid, 3-(dimethylamino)-1-methyl-3-oxo-1-propenyl dimethyl ester, (E)-	C ₉ H ₁₆ NO ₃ P 237.19	141-66-2	3077 400; 130 ^{0.1}	1.216 ¹⁵	
5173	Diethyl-ethyl Glycine, N-(chloroacetyl)-N-(2,6-diethylphenyl)-, ethyl ester	C ₁₉ H ₂₇ ClNO ₃ 311.81	38727-55-8			
5174	Difenocanazole cis,trans-3-Chloro-4-[4-methyl-2-(1H-1,2,4-triazol-1-ylmethyl)-1,3-dioxolan-2-yl]phenyl 4-chlorophenyl ether	C ₁₈ H ₁₇ Cl ₂ N ₃ O ₃ 406.27	119448-68-3 76	220 ^{0.60}		
5175	Difenzoquat methyl sulfate 1H-Pyrazolium, 1,2-dimethyl-3,5-diphenyl-, methyl sulfate	C ₁₇ H ₁₁ N ₃ Cl ₄ O ₆ S 380.43	43222-48-8 157			
5176	Difubenzuron Benzamide, N-[(4-chlorophenyl)amino]carbonyl-2,6-difluoro-	C ₁₄ H ₉ ClF ₂ N ₂ O ₂ 310.69	35387-36-5 239	3128		
5177	1,4:5,8-Dimethanonaphthalene, 1,2,3,4,10,10-hexachloro-1,4,4a,5,8,8a-hexahydro-, Aldrin	C ₁₂ H ₈ Cl ₆ 384.91	309-00-2 104	219	3-05-00-01365	H ₂ O 1; EtOH 3; eth 3; ace 3
5178	2,7:3,6-Dimethanonaphth[2,3-b]indirane, 3,4,5,6,8,9-hexachloro-1a,2,2a,3,8,8a,7,7a-octahydro-, (1a,2,2a,3,8,8a,7,7a)-Dieldrin	C ₁₂ H ₈ Cl ₆ O 380.81	60-57-1 175.5	3093	5-17-02-00087	H ₂ O 1; EtOH 2; ace 3; bz 3
5179	Dimethipin 2,3-Dihydro-5,8-dimethyl-1,4-dithiin, 1,1,4,4-tetraoxide	C ₈ H ₁₀ O ₄ S ₂ 210.28	55290-64-7 165		1.75 ²⁵	
5180	Dimethyl tetrachloroterephthalate 1,4-Benzenedicarboxylic acid, 2,3,5,6-tetrachloro-, dimethyl ester	C ₁₀ H ₆ Cl ₄ O ₄ 331.97	1881-32-1 155	2630		
5181	Dinitramine 1,3-Benzenediamine, N,N,N',N'-diethyl-2,4-dinitro-6-(trifluoromethyl)-	C ₁₁ H ₁₂ F ₃ N ₄ O ₄ 322.24	29081-05-2 96			
5182	Dinocap 2-Butenoic acid, 2-(1-methylheptyl)-4,6-dinitrophenyl ester	C ₁₉ H ₂₆ N ₂ O ₆ 364.40	6119-92-2	136 ^{0.01}		
5183	Dinosab Phenol, 2-(1-methylpropyl)-4,6-dinitro-	C ₁₀ H ₁₂ N ₂ O ₅ 240.22	88-85-7 40	3282	1.265 ⁴⁸	
5184	2,3-Dioxabicyclo[2.2.2]oct-5-ene, 1-methyl-4-(1-methylthio)- Ascaridole	C ₁₀ H ₁₆ O ₂ 168.24	512-85-8 3.3	852	5-19-01-00319	H ₂ O 1; EtOH 3; ace 3; bz 3
5185	1,7-Dioxadispiro[4.0.4.2]dodeca-3,8-diene-2,8-dione, trans- Anemonin	C ₁₀ H ₈ O ₄ 192.17	508-44-1 158	674	5-19-05-00101	chl 4
5186	1,3-Dioxane 1,3-Dioxacyclohexane	C ₄ H ₈ O ₂ 88.11	505-22-8 45	108.1	5-19-01-00011 1.0342 ²⁰	H ₂ O 5; EtOH 5; eth 5; ace 5 1.4185 ²⁰
5187	1,4-Dioxane 1,4-Dioxacyclohexane	C ₄ H ₈ O ₂ 88.11	123-91-1 11.8	3294 101.5	5-19-01-00016 1.0337 ²⁰	H ₂ O 5; EtOH 5; eth 5; ace 5 1.4224 ²⁰
5188	1,4-Dioxane, 2,3-dichloro-	C ₄ H ₆ Cl ₂ O ₂ 157.00	95-58-0 30	80-2 ¹⁰	4-19-00-00030 1.468 ²⁰	H ₂ O 1; eth 4; ace 4; bz 4 1.4928 ²⁰
5189	1,3-Dioxane, 2,4-dimethyl-	C ₆ H ₁₂ O ₂ 116.18	798-20-1	118.5	5-19-01-00072 0.9392 ²⁰	H ₂ O 2; acid 4 1.4136 ²⁰
5190	1,3-Dioxane-4,6-dione, 2,2-dimethyl- Meldrum's acid	C ₈ H ₈ O ₄ 144.13	2033-24-1 84	5696	5-19-05-00008	
5191	1,3-Dioxane-2-ethanol, 4-hydroxy-α,8-dimethyl- Paralidol	C ₈ H ₁₁ O ₄ 171.17	19404-07-0 90	90 ¹⁵	4-01-00-03987 1.116 ²⁰	H ₂ O 4; eth 4; EtOH 4 1.4510 ²⁰
5192	1,4-Dioxane, 2,2,3,3,5,5,6-heptachloro- 1,4-Dioxane, heptachloro	C ₄ HCl ₇ O ₂ 329.22	6629-66-5 55	123-8 ⁸	4-19-00-00032	H ₂ O 1; eth 4; ace 4; bz 4
5193	1,3-Dioxane, 4-methyl-	C ₅ H ₁₀ O ₂ 102.13	1120-97-4 44.5	114	5-19-01-00054 0.9756 ²⁰	H ₂ O 2; bz 4 1.4159 ²⁰
5194	1,3-Dioxane, 4-methyl-4-phenyl- m-Dioxane, 4-methyl-4-phenyl-	C ₁₁ H ₁₄ O ₂ 178.23	1200-73-3 37.5	256	5-19-01-00481 1.0684 ²⁰	H ₂ O 1; chl 2; os 3 1.5240 ²⁰
5195	1,3-Dioxane, 2-phenyl-	C ₁₀ H ₁₂ O ₂ 164.20	772-01-0 41	253	5-19-01-00459 1.6053 ²⁰	EtOH 4; eth 4
5196	1,3-Dioxane, 4-phenyl-	C ₁₀ H ₁₂ O ₂ 164.20	772-00-8	247	5-19-01-00464 1.1036 ²⁰	H ₂ O 1; os 3 1.5308 ¹⁸
5197	1,3-Dioxan-5-ol, 2-methyl-	C ₇ H ₁₀ O ₃ 118.13	3774-03-6	178; 79 ¹⁸	4-19-00-00624 1.0705 ¹⁷	H ₂ O 4 1.4375 ¹⁷
5198	1,3,2-Dioxathiane, 4-methyl-, 2-oxide 1,3-Butanedithiol, sulfite	C ₄ H ₆ O ₃ S 138.17	4428-51-1 5	165	4-01-00-02510 1.2352 ²⁰	EtOH 4; eth 4; ace 4; bz 4 1.4881 ²⁰

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PHYSICAL CONSTANTS OF ORGANIC COMPOUNDS (continued)

No.	Name Synonym	Mol. Form. Mol. Wt.	CAS RN mp/°C	Merck No. bp/°C	Boil. Ref. dens/g cm ⁻³	Solubility n _D
8964	2-Pentanone, 5-(diethylamino)-	C ₉ H ₁₉ NO 157.28	105-14-6	83-515	4-04-00-01935 0.88125	1.435020
8965	2-Pentanone, 4,4-dimethyl-	C ₇ H ₁₄ O 114.19	590-50-1 -64	126	4-01-00-03331 0.80925	1.403620
8966	3-Pentanone, 2,2-dimethyl- 2,2-Dimethyl-3-pentanone	C ₇ H ₁₄ O 114.19	584-04-5 -45	125.6	4-01-00-03331 0.812520	H ₂ O 2; EtOH 3; eth 3; ace 3 1.406520
8967	3-Pentanone, 2,4-dimethyl- Diisopropyl ketone	C ₇ H ₁₄ O 114.19	565-80-0 -69	125.4	4-01-00-03334 0.810820	H ₂ O 1; EtOH 5; eth 5; bz 3 1.399920
8968	3-Pentanone, 2,4-dimethyl-, oxime Diisopropyl ketone oxime	C ₇ H ₁₅ NO 129.20	1113-74-2 34	181; 91.521	4-01-00-03335 0.902217	
8969	3-Pentanone, 1,5-diphenyl- Diphenethyl ketone	C ₁₇ H ₁₆ O 238.33	5396-91-8 13.5	352	4-07-00-01482 1.03560	
8970	2-Pentanone, 3-ethyl-4-methyl-	C ₈ H ₁₆ O 128.21	71172-57-1	154.5	3-01-00-02883 0.81220	H ₂ O 3; EtOH 5; eth 5; bz 5 1.410520
8971	2-Pentanone, 1-hydroxy- 1-Pentanol-2-one	C ₅ H ₁₀ O ₂ 102.13	64502-69-2	152	4-01-00-04004 0.988020	H ₂ O 4; eth 4; EtOH 4 1.423412
8972	2-Pentanone, 3-hydroxy-	C ₅ H ₁₀ O ₂ 102.13	3142-68-3	147.5	3-01-00-03220 0.950020	H ₂ O 4; ace 4; bz 4; eth 4 1.435010
8973	2-Pentanone, 4-hydroxy-	C ₅ H ₁₀ O ₂ 102.13	4161-80-6	177	4-01-00-04005 1.007120	H ₂ O 3; EtOH 3; eth 3 1.441518
8974	2-Pentanone, 5-hydroxy-	C ₅ H ₁₀ O ₂ 102.13	1071-73-4	209; 11733	4-01-00-04006 1.007120	H ₂ O 5; EtOH 3; eth 3 1.439020
8975	3-Pentanone, 2-hydroxy- 2-Pentanol-3-one	C ₅ H ₁₀ O ₂ 102.13	5704-20-1	152.5	4-01-00-04008 0.974220	eth 4; EtOH 4 1.412820
8976	2-Pentanone, 4-hydroxy-4-methyl- Diacetone alcohol	C ₈ H ₁₂ O ₂ 118.16	123-42-2 -44	2944 167.9	4-01-00-04023 0.936720	H ₂ O 5; EtOH 5; eth 5; chl 3 1.421320
8977	2-Pentanone, 4-amino-	C ₅ H ₉ NO 98.13	870-74-8 43	209	4-01-00-03678 0.94270	H ₂ O 4; eth 4
8978	2-Pentanone, 4-methoxy-4-methyl- Pentoxone	C ₇ H ₁₄ O ₂ 130.19	107-70-0	160	4-01-00-04024 0.898025	1.41820
8979	1-Pentanone, 1-(3-methoxyphenyl)-	C ₁₂ H ₁₆ O ₂ 182.26	20359-55-1	19630	4-08-00-00533 1.01220	1.524231
8980	2-Pentanone, 3-methyl-, (s)- 2-Pentanone, 3-methyl (DL)	C ₈ H ₁₆ O 100.16	55156-16-6	118	4-01-00-03309 0.813020	H ₂ O 2; EtOH 5; eth 5; chl 3 1.400220
8981	2-Pentanone, 4-methyl- Isobutyl methyl ketone	C ₈ H ₁₆ O 100.16	108-10-1 -84	5095 118.5	4-01-00-03305 0.797820	H ₂ O 2; EtOH 5; eth 5; ace 5 1.396220
8982	3-Pentanone, 2-methyl- Ethyl isopropyl ketone	C ₈ H ₁₆ O 100.16	565-69-5	113.5	4-01-00-03304 0.81418	H ₂ O 2; EtOH 4; eth 5; ace 5 1.397520
8983	1-Pentanone, 4-methyl-1-phenyl-	C ₁₂ H ₁₈ O 178.28	2050-07-9 -2	255.5	3-07-00-01158 0.962315	ace 4; bz 4; eth 4; EtOH 4 1.53320
8984	2-Pentanone, 3-methyl-1-phenyl- Benzyl sec-butyl ketone	C ₁₂ H ₁₈ O 178.28	27893-42-6	127-617	4-07-00-00758 0.98420	1.501820
8985	2-Pentanone, oxime Methyl propyl ketone oxime	C ₅ H ₁₁ NO 101.15	823-40-5	188	4-01-00-03274 0.909520	H ₂ O 4; eth 4; EtOH 4 1.445020
8986	1-Pentanone, 1-phenyl-	C ₁₁ H ₁₄ O 162.23	1009-14-9 -94	245	4-07-00-00733 0.88620	H ₂ O 1; EtOH 4; eth 4; ctc 2 1.515820
8987	2-Pentanone, 3-(phenyl(methylene)- Methyl α-ethylstyryl ketone	C ₁₂ H ₁₄ O 174.24	3437-89-8	136-612	3-07-00-01461 1.000522	1.585022
8988	3-Pentanone, 2,2,4,4-tetramethyl-	C ₉ H ₁₈ O 142.24	815-24-7 -25.2	152	4-01-00-03365 0.824018	H ₂ O 1; EtOH 3; eth 3; ace 3 1.419420
8989	3-Pentanone, 2,2,4-trimethyl- tert-Butyl isopropyl ketone	C ₉ H ₁₈ O 128.21	5857-38-3	135.1	4-01-00-03351 0.806520	H ₂ O 1; eth 3; ace 3 1.4060
8990	Pentanoyl chloride Valeroyl chloride	C ₅ H ₉ ClO 120.58	638-29-9 -110	109	4-02-00-00874 1.015515	1.420020
8991	Pentanoyl chloride, 2-chloro-	C ₅ H ₉ Cl ₂ O 155.02	61589-68-2	156	4-02-00-00879 1.176520	eth 4 1.448520
8992	Pentanoyl chloride, 5-chloro-	C ₅ H ₉ Cl ₂ O 155.02	1575-81-7	6312	4-02-00-00881 1.21018	eth 4 1.463920
8993	Pentanoyl chloride, 2-methyl-, (s)- Valeryl chloride, 2-methyl (DL)	C ₆ H ₁₁ ClO 134.61	118908-84-0	141	3-02-00-00741 0.978120	eth 4 1.433027
8994	Pentanoyl chloride, 3-methyl-, (s)- Valeryl chloride, 3-methyl (DL)	C ₆ H ₁₁ ClO 134.61	118908-85-1	141	4-02-00-00949 0.978120	eth 4
8995	2,5,8,11,14-Pentaoxapentadecane Tetraethylene glycol dimethyl ether	C ₁₀ H ₂₂ O ₅ 222.28	143-24-6	9141 275.3	4-01-00-02404 1.011420	H ₂ O 5; EtOH 3; eth 3; ctc 3 1.419420
8996	Pentaphene 2,3,6,7-Dibenzphenanthrene	C ₂₂ H ₁₄ 278.35	222-93-5 257	2892	4-05-00-02721	H ₂ O 1; EtOH 2; eth 2; bz 3
8997	Pentasiloxane, dodecamethyl- Dodecamethylpentasiloxane	C ₁₂ H ₂₆ O ₄ Si ₅ 384.84	141-63-8 -80	3401 232; 10512	4-04-00-04124 0.875520	ctc 3; CS ₂ 3 1.392520
8998	1,2,3,5,8-Pentathiepane Lanthionine	C ₅ H ₈ S ₅ 168.36	282-48-6 60.5	5321	5-19-12-00251	
8999	Pentatriacontane	C ₃₅ H ₇₂ 492.96	630-07-9 75	490	4-01-00-00598 0.815720	H ₂ O 1; eth 2; ace 3 1.456820
9000	16-Pentatriacontanone	C ₃₅ H ₇₀ O 506.94	504-53-0 89.0	2700.1	4-01-00-03413 0.79395	H ₂ O 1; EtOH 2; eth 2; ace 2
9001	4-Pentenal Pent-4-en-1-al	C ₅ H ₈ O 84.12	2100-17-6	99	4-01-00-03458 0.85220	H ₂ O 1; eth 3; ace 3 1.419120
9002	2-Pentenal, 2-methyl-	C ₆ H ₁₀ O 98.14	623-38-9	138.5	4-01-00-03471 0.858120	H ₂ O 1; EtOH 3; eth 3; bz 3 1.448820
9003	4-Pentanamide, 2,2-diethyl- Novonol	C ₉ H ₁₇ NO 155.24	512-48-1 75.5	6843	3-02-00-01351	eth 4; EtOH 4