

**Safety Data Sheet**  
according to Regulation (EC) No. 1907/2006 (REACH)



**Trade name :** ORINOX  
**Revision date :** 07.03.2014  
**Print date :** 26-05-2015

**Version (Revision) :** 1.1.6 (1.1.5)

**SECTION 1: Identification of the substance/mixture and of the company/undertaking**

**1.1 Product identifier**

ORINOX (W00836)  
4'-tert-butyl-2',6'-dimethylacetophenone ; CAS No. : 2040-10-0 ; EC No. : 218-037-8

**1.2 Relevant identified uses of the substance or mixture and uses advised against**

**Relevant identified uses**

Fragrance ingredient which may be used in fragrance compounds according to the current legislation and IFRA rules.  
Reserved for industrial and professional use.

**Uses advised against**

Not intended for oral consumption.

**1.3 Details of the supplier of the safety data sheet**

**Supplier (manufacturer/importer/only representative/downstream user/distributor)**

PFW Aroma Chemicals B.V.

**Street :** Veemweg 29-31

**Postal code/city :** NL - 3371 MT Barneveld

**Telephone :** +31 342 40 77 00

**Telefax :** +31 342 40 77 20

**Information contact :** pfw@pfw.nl

**1.4 Emergency telephone number**

+31 342 40 77 93

**SECTION 2: Hazards identification**

**2.1 Classification of the substance or mixture**

**Classification according to Regulation (EC) No. 1272/2008 [CLP]**

Acute Tox. 4 ; H312 - Acute toxicity (dermal) : Category 4 ; Harmful in contact with skin.

Acute Tox. 3 ; H301 - Acute toxicity (oral) : Category 3 ; Toxic if swallowed.

**Hazard classes and hazard categories**

Acute Tox. 3 (Oral) ; Acute Tox. 4 (Dermal)

**Classification according to Directive 67/548/EEC or 1999/45/EC**

Harmful in contact with skin and if swallowed.

Xn ; R 21/22

**2.2 Label elements**

**Labelling according to Regulation (EC) No. 1272/2008 [CLP]**

**Hazard pictograms**



Skull and crossbones (GHS06)

**Signal word**

Danger

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## Hazard statements

H301 Toxic if swallowed.  
H312 Harmful in contact with skin.

## Precautionary statements

P280 Wear protective gloves/protective clothing/eye protection/face protection.  
P301+P310 IF SWALLOWED: Immediately call a POISON CENTER / doctor.  
P302+P352 IF ON SKIN: Wash with plenty of water.  
P391 Collect spillage.  
P405 Store locked up.  
P501 Dispose of contents/container to a chemical waste treatment facility or recycling plant.

## 2.3 Other hazards

None

## SECTION 3: Composition / information on ingredients

### 3.1 Substances

**Substance name :** 4'-tert-butyl-2',6'-dimethylacetophenone

**EC No. :** 218-037-8

**CAS No. :** 2040-10-0

**Purity :** ≥ 99 % [mass]

#### Synonymes

**IUPAC :** 1-(4-tert-Butyl-2,6-dimethylphenyl)ethanone

**INCI :** TERT-BUTYL DIMETHYL ACETOPHENONE

## SECTION 4: First aid measures

### 4.1 Description of first aid measures

#### General information

Medical examination necessary even merely on suspicion of intoxication. Remove victim out of the danger area. Put victim at rest, cover with a blanket and keep warm. Do not leave affected person unattended. If unconscious place in recovery position and seek medical advice.

#### In case of inhalation

Remove casualty to fresh air and keep warm and at rest. If breathing is irregular or stopped, administer artificial respiration.

#### In case of skin contact

Change contaminated, saturated clothing. After contact with skin, wash immediately with plenty of water and soap. Call a physician immediately. Water Do not wash with: Solvents/Thinner

#### After eye contact

In case of contact with eyes flush immediately with plenty of flowing water for 10 to 15 minutes holding eyelids apart and consult an ophthalmologist.

#### After ingestion

Rinse mouth thoroughly with water. Call a physician in any case! Let water be drunken in little sips (dilution effect). Do NOT induce vomiting.

### 4.2 Most important symptoms and effects, both acute and delayed

No information available.

### 4.3 Indication of any immediate medical attention and special treatment needed

None

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## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

alcohol resistant foam. Extinguishing powder. Water mist

#### Unsuitable extinguishing media

Strong water jet.

### 5.2 Special hazards arising from the substance or mixture

#### Hazardous combustion products

In case of fire may be liberated: Carbon dioxide (CO<sub>2</sub>) Carbon monoxide (CO).

### 5.3 Advice for firefighters

Do not inhale explosion and combustion gases. Use water spray jet to protect personnel and to cool endangered containers. Do not allow run-off from fire-fighting to enter drains or water courses.

#### Special protective equipment for firefighters

Wear a self-contained breathing apparatus and chemical protective clothing.

## SECTION 6: Accidental release measures

### 6.1 Personal precautions, protective equipment and emergency procedures

Do not breathe dust. Provide adequate ventilation. Remove persons to safety. See protective measures under point 7 and 8.

### 6.2 Environmental precautions

Ensure all waste water is collected and treated via a waste water treatment plant. In case of entry into waterways, soil or drains, inform the responsible authorities.

### 6.3 Methods and material for containment and cleaning up

Wet clean or vacuum up solids. Avoid generation of dust. Collect in closed and suitable containers for disposal.

### 6.4 Reference to other sections

See protective measures under point 7 and 8.

## SECTION 7: Handling and storage

### 7.1 Precautions for safe handling

When using do not eat, drink, smoke, sniff. Wash hands before breaks and after work. Provide adequate ventilation as well as local exhaust at critical locations. All work processes must always be designed so that the following is as low as possible: eye contact, skin contact. In case of entry into waterways, soil or drains, inform the responsible authorities. Wear personal protection equipment (see chapter 8).

#### Protective measures

##### Specific requirements or handling rules

Melt completely before use!

### 7.2 Conditions for safe storage, including any incompatibilities

#### Technical measures and storage conditions

Ensure adequate ventilation of the storage area. Keep/Store only in original container. Use isolated drainage to prevent discharge to soil. Restrict access to stockrooms. Keep the packing dry and well sealed to prevent contamination and absorption of humidity. Never use pressure to empty container.

#### Hints on joint storage

Keep away from oxidising agent, acid and alkali.

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Storage class : 13  
Storage class (TRGS 510) : 6.1C

7.3 Specific end use(s)  
None

## SECTION 8: Exposure controls/personal protection

### 8.1 Control parameters

To date, no national critical limit values exist.

### 8.2 Exposure controls

When using do not eat, drink, smoke, sniff. Wash hands before breaks and after work.

#### Appropriate engineering controls

Provide adequate ventilation as well as local exhaust at critical locations. If technical exhaust or ventilation measures are not possible or insufficient, respiratory protection must be worn.

#### Personal protection equipment

##### Eye/face protection

Eye glasses with side protection

##### Skin protection

###### Hand protection

Gloves. The quality of the protective gloves resistant to chemicals must be chosen as a function of the specific working place concentration and quantity of hazardous substances. Breakthrough times and swelling properties of the material must be taken into consideration.

**Suitable material** : Butyl caoutchouc (butyl rubber)

**Breakthrough time (maximum wearing time)** : >480 min.

**Thickness of the glove material** : 1.00 mm.

**Recommended glove articles** : Butyl Plus/R0,5

###### Body protection

Overall

##### Respiratory protection

Respiratory protection necessary at: exceeding exposure limit values Mask type: filtering face piece (FFP2) Container device with compressed air (DIN EN 137) / Filtering device (full mask or mouthpiece) with filter: Filter types:A, B, E, K. Class 1: Maximum permitted contaminant concentration in inhaled air = 1000 mL/m<sup>3</sup> (0.1 % by vol.); class 2: maximum permitted contaminant concentration in inhaled air = 5000 mL/m<sup>3</sup> (0.5 % by vol.); class 3: maximum permitted contaminant concentration in inhaled air = 10000 mL/m<sup>3</sup> (1.0 % by vol.)

#### General health and safety measures

Full-face mask or mouthpiece with particulate filter: maximum use concentration for substances with exposure limits: P1 filter: up to a max. of 4 times the exposure limit. P2 filter: up to a max. of 15 times the exposure limit. P3 filter: up to a max. of 400 times the exposure limit.

#### Environmental exposure controls

Send to a hazardous waste incinerator facility under observation of official regulations.

## SECTION 9: Physical and chemical properties

### 9.1 Information on basic physical and chemical properties

**Odour threshold in air** : No data available

#### Safety relevant basis data

**Physical state** :

solid

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Colour :			off-white to yellow	
Odour :			musky	
Melting point/melting range :	( 1013 hPa )	>	47 °C	
Boiling temperature/boiling range :	( 1013 hPa )	ca.	280 °C	
Decomposition temperature :	( 1013 hPa )		No data available	
Flash point (Closed Cup) :		>	100 °C	DIN EN 51578
Flammability (solid, gas) :			none	
Auto-ignition temperature :			no data available	
Evaporation rate :			slowly evaporating	
Lower explosion limit :			No data available	
Upper explosion limit :			No data available	
Explosive properties :			none	
Vapour pressure :	( 50 °C )	ca.	0,05 hPa	
Surface tension (20°C)	( 20 °C )		not applicable	
Vapour Density	( 25 °C )		1	
Density :	( 20 °C )		0,9 g/cm <sup>3</sup>	
Water solubility :			slightly soluble (0.1-100 mg/l)	
pH value :			not applicable	
Log Pow :			4,7	
Viscosity :	( 20 °C )		not applicable	
Oxidising properties :			none	
Refractive Index			not applicable	

## 9.2 Other information

Justification for data waiving. . pH value: The substance is not soluble in water. Surface tension: : The substance is not soluble in water. Viscosity: : Testing can be waived because substance is a solid. Refractive index: : Testing can be waived because substance is a solid.

## SECTION 10: Stability and reactivity

### 10.1 Reactivity

No known hazardous reactions.

### 10.2 Chemical stability

The product is stable under storage at normal ambient temperatures.

### 10.3 Possibility of hazardous reactions

No hazardous reaction when handled and stored according to provisions.

### 10.4 Conditions to avoid

Do not expose to temperatures above 40°C in the original container.

### 10.5 Incompatible materials

Exothermic reaction with: oxidising agent strong acid strong alkali

### 10.6 Hazardous decomposition products

Decomposition with: Carbon dioxide (CO<sub>2</sub>). Carbon monoxide (CO).

## SECTION 11: Toxicological information

### 11.1 Information on toxicological effects

#### Acute effects

##### Acute oral toxicity

Parameter : LD50 ( 4'-tert-butyl-2',6'-dimethylacetophenone ; CAS No. : 2040-10-0 )

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Exposure route : Oral  
Species : Rat  
Effective dose : 260 mg/kg  
Exposure time : 15 days  
Methode : OECD 401 Acute Oral Toxicity  
Source : PFW Aroma Chemicals BV

### Acute dermal toxicity

Parameter : LD50 ( 4'-tert-butyl-2',6'-dimethylacetophenone ; CAS No. : 2040-10-0 )  
Exposure route : Dermal  
Species : Rat  
Effective dose : 1100 mg/kg  
Exposure time : 3 days  
Methode : OECD 402  
Source : PFW Aroma Chemicals BV

### Irritant and corrosive effects

#### Primary irritation to the skin

Parameter : Irritation of the skin ( 4'-tert-butyl-2',6'-dimethylacetophenone ; CAS No. : 2040-10-0 )  
Parameter : Rabbit  
Result : No Irritation  
Methode : OECD 404 Acute Dermal Irritation/Corrosion  
Source : PFW Aroma Chemicals BV

## SECTION 12: Ecological information

### 12.1 Toxicity

No information available.

### 12.2 Persistence and degradability

#### Biodegradation

Analytical method : Biodegradation ( 4'-tert-butyl-2',6'-dimethylacetophenone ; CAS No. : 2040-10-0 )  
Evaluation : Not readily biodegradable (according to OECD criteria)  
Methode : QSAR  
Source : PFW Aroma Chemicals BV

### 12.3 Bioaccumulative potential

Parameter : Bioconcentration factor (BCF) ( 4'-tert-butyl-2',6'-dimethylacetophenone ; CAS No. : 2040-10-0 )  
Result : ca. 150 l/kg ww  
Methode : QSAR  
Source : PFW Aroma Chemicals BV  
Parameter : Partition coefficient n-octanol /water (log P O/W) ( 4'-tert-butyl-2',6'-dimethylacetophenone ; CAS No. : 2040-10-0 )  
Result : ca. 4,7  
Methode : QSAR  
Source : PFW Aroma Chemicals BV

Based on the n-octanol/water partition coefficient accumulation in organisms is possible.

### 12.4 Mobility in soil

No information available.

### 12.5 Results of PBT and vPvB assessment

This substance does not meet the PBT/vPvB criteria of REACH, annex XIII.

### 12.6 Other adverse effects

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No information available.

## 12.7 Further ecological information

None

## SECTION 13: Disposal considerations

### 13.1 Waste treatment methods

Send to a hazardous waste incinerator facility under observation of official regulations.

## SECTION 14: Transport information

### 14.1 UN number

UN 2811

### 14.2 UN proper shipping name

#### Land transport (ADR/RID)

TOXIC SOLID, ORGANIC, N.O.S. ( t-butyl dimethylacetophenone )

#### Sea transport (IMDG)

TOXIC SOLID, ORGANIC, N.O.S. ( t-butyl dimethylacetophenone )

#### Air transport (ICAO-TI / IATA-DGR)

TOXIC SOLID, ORGANIC, N.O.S. ( t-butyl dimethylacetophenone )

### 14.3 Transport hazard class(es)

#### Land transport (ADR/RID)

Class(es) : 6.1  
Classification code : T2  
Hazard identification number (Kemler No.) : 60  
Tunnel restriction code : E  
Special provisions : LQ 5 kg · E 1  
Hazard label(s) : 6.1

#### Sea transport (IMDG)

Class(es) : 6.1  
EmS-No. : F-A / S-A  
Special provisions : LQ 5 kg · E 1 · Segregation Group: No/none  
Hazard label(s) : 6.1

#### Air transport (ICAO-TI / IATA-DGR)

Class(es) : 6.1  
Special provisions : E 1  
Hazard label(s) : 6.1

### 14.4 Packing group

III

### 14.5 Environmental hazards

Land transport (ADR/RID) : No

Sea transport (IMDG) : No

Air transport (ICAO-TI / IATA-DGR) : No

### 14.6 Special precautions for user

None

## SECTION 15: Regulatory information

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### 15.1 Safety, health and environmental regulations/legislation specific for the substance or mixture

#### National regulations

##### Water hazard class (WGK)

Class : strongly water pollutant according VwVwS

##### Other regulations, restrictions and prohibition regulations

TSCA (USA) : listed

CEPA (Canada) : NDSL

Asia-PAC : listed

India : not applicable

ENCS (Japan) : listed 3 - 1254

IECSC (China) : listed

CSNN (Taiwan) : listed

ECL (Korea) : not listed

PICCS (Philippines) : listed

AICS (Australia) : listed

NZIoC (New Zealand) : listed

FLAVIS (EU) : not listed

CoE (EU) : not listed

JECFA (UN) : not listed

FEMA (USA) : not listed

GRAS (USA) : not listed

### 15.2 Chemical Safety Assessment

Chemical safety assessments for substances in this mixture were not carried out.

## SECTION 16: Other information

### 16.1 Indication of changes

None

### 16.2 Abbreviations and acronyms

a.i. = Active ingredient; ACGIH = American Conference of Governmental Industrial Hygienists (US); ADR = European Agreement concerning the International Carriage of Dangerous Goods by Road; AFFF = Aqueous Film Forming Foam; AICS = Australian Inventory of Chemical Substances; AISE = International Association for Soaps, Detergents and Maintenance Products (joint project of AISE and CEFIC); AOAC = AOAC International (formerly Association of Official Analytical Chemists); aq. = Aqueous; Asia-PAC = Asia Pacific; ASTM = American Society of Testing and Materials (US); atm = Atmosphere(s); B.V. = Beperkt Vennootschap (LTD = Limited); BCF = Bioconcentration Factor; bp = Boiling point at stated pressure; bw = Body weight; ca = (Circa) about; CAS No = Chemical Abstracts Service Number (see ACS - American Chemical Society); CEFIC = European Chemical Industry Council (established 1972); CEPA = Canadian Environmental Protection Act (CAN); CEPA = Canadian Environmental Protection Act (Canada); CIPAC = Collaborative International Pesticides Analytical Council; CLP = REGULATION (EC) No 1272/2008 on classification, labelling and packaging of substances and mixtures.; CoE = Council of Europe (EU); Conc = Concentration; cP = CentiPoise; CSNN = Chemical Substance Nomination & Notification (Taiwan); cSt = Centistokes; d = Day(s); DIN = Deutsches Institut für Normung e.V.; DNEL = Derived No-Effect Level; DSL = Domestic Substances List; DT50 = Time for 50% loss; half-life; EbC50 = Median effective concentration (biomass, e.g. of algae); EC = European Community; European Commission; EC50 = Median effective concentration; ECL = Existing Chemicals List (Korea); EINECS = European Inventory of Existing Commercial Chemical Substances (EU, outdated, now replaced by EC Number); ELINCS = European List of Notified (New) Chemicals; ENCS = Existing and New Chemical Substances Inventory (Japan); ErC50 = Median effective concentration (growth rate, e.g. of algae); EU = European Union; EWC = European Waste Catalogue; FAO = Food and Agriculture Organization (United Nations); FEMA = Flavor & Extract Manufacturers Association (USA); FLAVIS = Flavour Information System (EU); GIFAP = Groupement International des Associations Nationales de Fabricants de Produits



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Agrochimiques (now CroLife International); GRAS = Generally Recognized As Safe (USA); h = Hour(s); hPa = HectoPascal (unit of pressure); IARC = International Agency for Research on Cancer; IATA = International Air Transport Association; IC50 = Concentration that produces 50% inhibition; IECSC = Inventory of Existing Chemical Substances (China); IMDG Code = International Maritime Dangerous Goods Code; IMO = International Maritime Organization; ISO = International Organization for Standardization; IUCLID = International Uniform Chemical Information Database; IUPAC = International Union of Pure and Applied Chemistry; IVIS = In-Vitro Irritancy Score; JECFA = Joint Expert Committee on Food Additives (United Nations); kg = Kilogram; Kow = Distribution coefficient between n-octanol and water; kPa = KiloPascal (unit of pressure); LC50 = Concentration required to kill 50% of test organisms; LD50 = Dose required to kill 50% of test organisms; LEL = Lower Explosive Limit/Lower Explosion Limit; LOAEL = Lowest observed adverse effect level; LVE = Low Volume Exemption; mg = Milligram; min = Minute(s); ml = Milliliter; mmHg = Pressure equivalent to 1 mm of mercury (133.3 Pa); mp = Melting point; MRL = Maximum Residue Limit; MSDS = Material Safety Data Sheet; n.o.s. = Not Otherwise Specified; NDSL = Non-Domestic Substances List; NIOSH = National Institute for Occupational Safety and Health (US); NOAEL = No Observed Adverse Effect Level; NOEC = No observed effect concentration; NOEL = No Observable Effect Level; NOx = Oxides of Nitrogen; NZIoC = New Zealand Inventory of Chemicals; OECD = Organization for Economic Cooperation and Development; OEL = Occupational Exposure Limits; Pa = Pascal (unit of pressure); PBT = Persistent, Bioaccumulative or Toxic; pH = -log10 hydrogen ion concentration; PICCS = Philippine Inventory of Chemicals and Chemical Substances; pKa = -log10 acid dissociation constant; PNEC = Predicted No Effect Concentration; POPs = Persistent Organic Pollutants; ppb = Parts per billion; PPE = Personal Protection Equipment; ppm = Parts per million; ppt = Parts per trillion; PVC = Polyvinyl Chloride; QSAR = Quantitative Structure-Activity Relationship; REACH = Registration, Evaluation and Authorization of Chemicals (EU, see NCP); SI = International System of Units; STEL = Short-Term Exposure Limit; tech. = Technical grade; TSCA = Toxic Substances Control Act (US); TSCA = Toxic Substances Control Act (USA); TWA = Time-Weighted Average; UN = United Nations; vPvB = Very Persistent and Very Bioaccumulative; VwVwS = Verwaltungsvorschrift wassergefährdender Stoffe; WHO = World Health Organization = OMS; y = Year(s);

### 16.3 Key literature references and sources for data

None

### 16.4 Relevant R-, H- and EUH-phrases (Number and full text)

H301	Toxic if swallowed.
H312	Harmful in contact with skin.
21/22	Harmful in contact with skin and if swallowed.

### 16.5 Training advice

None

### 16.6 Additional information

None

The above information describes exclusively the safety requirements of the product and is based on our present-day knowledge. The information is intended to give you advice about the safe handling of the product named in this safety data sheet, for storage, processing, transport and disposal. The information cannot be transferred to other products. In the case of mixing the product with other products or in the case of processing, the information on this safety data sheet is not necessarily valid for the new made-up material.