I U C L I D

D a t a s e t

Existing Chemical	Substance ID: 98–86–2
CAS No.	98–86–2
EINECS Name	acetophenone
EINECS No.	202–708–7
Molecular Formula	C8H8O

Dataset created by: EUROPEAN COMMISSION – European Chemicals Bureau

This dossier is a compilation based on data reported by the European Chemicals Industry following 'Council Regulation (EEC) No. 793/93 on the Evaluation and Control of the Risks of Existing Substances'. All (non–confidential) information from the single datasets, submitted in the IUCLID/HEDSET format by individual companies, was integrated to create this document.

The data have not undergone any evaluation by the European Commission.

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1.0.1 OECD and Company Information

Name: Enichem S.p.A.
Street: Via Taramelli,26
Town: 20124 Milan
Country: Italy

Name: Phenolchemie GmbH
Street: Dechenstr. 3
Town: 45966 Gladbeck
Country: Germany
Phone: 02043/58-0
Telefax: 02043/52227
Telex: 8579219

Name: Rhodia Chimie
Street: 25, Quai Paul Doumer
Town: 92408 COURBEVOIE
Country: France
Telex: 01 47 68 12 34

Name: Ruetgerswerke AG
Street: Varziner Str. 49
Town: 47138 Duisburg
Country: Germany

1.0.2 Location of Production Site

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1.0.3 Identity of Recipients

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1.1 General Substance Information

Substance type: organic
Physical status: liquid

1.1.1 Spectra

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1.2 Synonyms

1-Phenylethanone
Source: Rhodia Chimie COURBEVOIE

Acetylbenzene
Source: Rhodia Chimie COURBEVOIE
Phenolchemie GmbH Gladbeck
Ruetgerswerke AG Duisburg

acetylbenzene;methyl phenyl ketone;1-phenylethanone;benzoyl methide
Source: Enichem S.p.A. Milan

Hypnone
Source: Phenolchemie GmbH Gladbeck
Ruetgerswerke AG Duisburg

Methyl phenyl cetone
Source: Rhodia Chimie COURBEVOIE

Methylphenylketone
Source: Phenolchemie GmbH Gladbeck
Ruetgerswerke AG Duisburg

Phenylethanone
Source: Phenolchemie GmbH Gladbeck
Ruetgerswerke AG Duisburg

Phenylmethylketone
Source: Phenolchemie GmbH Gladbeck
Ruetgerswerke AG Duisburg

1.3 Impurities

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1.4 Additives

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1.5 Quantity

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1.6.1 Labelling

Labelling: as in Directive 67/548/EEC
Symbols: Xn
D
Specific limits: no data
R-Phrases: (22) Harmful if swallowed
(36) Irritating to eyes
S-Phrases: (2) Keep out of reach of children
(26) In case of contact with eyes, rinse immediately with plenty of water and seek medical advice

1.6.2 Classification

Classification: as in Directive 67/548/EEC
Class of danger: corrosive
R–Phrases: (22) Harmful if swallowed

Classification: as in Directive 67/548/EEC
Class of danger: irritating
R–Phrases: (36) Irritating to eyes

1.7 Use Pattern

Type: type
Category: Non dispersive use

Type: type
Category: Use in closed system

Type: type
Category: Wide dispersive use

Type: industrial
Category: Basic industry: basic chemicals

Type: industrial
Category: Chemical industry: used in synthesis

Type: industrial
Category: Paints, lacquers and varnishes industry

Type: industrial
Category: Polymers industry

Type: use
Category: Intermediates

Type: use
Category: Solvents

Type: use
Category: other: Perfumery

Type: use
Category: other: plasticizers; solvent industry; resins

Type: use
Category: other: polymeric additives

1.7.1 Technology Production/Use

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1.8 Occupational Exposure Limit Values

Type of limit: TLV (US)
Limit value: 49 mg/m3
Source: Enichem S.p.A. Milan

(1)

1.9 Source of Exposure

Remark: Natural occuring sources : in oil of labdanum, stirlingea latifolia, urtica dioica, elsholtzia argyi var nipponica, elisholtzia ciliata, in various species of orthodon (o citraliferum o linalooliferum var laerolinoloolliferum o linaloiferum o sabinoliferum var taiwanese), & in castoreum absulute...
Source: Enichem S.p.A. Milan

(2)

Remark: Artificial Sources: In gasoline exhaust: <0.1 to 0.4 ppm
Source: Enichem S.p.A. Milan

(3)

Remark: Production process: obtained as by-product in the Phenol manufacturing
Source: Enichem S.p.A. Milan

(4)

Remark: Acetophenone is produced by distillation of residues of the Hock synthesis of phenol.
Source: Ruetgerswerke AG Duisburg

1.10.1 Recommendations/Precautionary Measures

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1.10.2 Emergency Measures

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1.11 Packaging

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1.12 Possib. of Rendering Subst. Harmless

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1.13 Statements Concerning Waste

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1.14.1 Water Pollution

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1.14.2 Major Accident Hazards

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1.14.3 Air Pollution

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1.15 Additional Remarks

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1.16 Last Literature Search

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1.17 Reviews

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1.18 Listings e.g. Chemical Inventories

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2.1 Melting Point

Value: 19.7 degree C
Method: other
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(5)

Value: 20 degree C
Method: other
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(6)

Value: 20.5 degree C
Method: other
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(7)

2.2 Boiling Point

Value: 201.7 degree C at 1013 hPa
Method: other
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(5)

Value: 202 degree C at 1013 hPa
Method: other
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(6)

Value: 202.6 degree C at 1013 hPa
Method: other
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(7)

2.3 Density

Type: relative density
Value: 1.0281 at 20 degree C
Method: other
GLP: no data
Remark: relative to water at 4 degree C
Source: Phenolchemie GmbH Gladbeck
(7)

Type: relative density
Value: 1.03 at 20 degree C
Method: other
GLP: no data
Remark: relative to water at 20 degree C
Source: Phenolchemie GmbH Gladbeck

(5)

2.3.1 Granulometry

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2.4 Vapour Pressure

Value: 1.33 hPa at 15 degree C
Method: other (measured)
GLP: no data
Source: Phenolchemie GmbH Gladbeck

(8)

2.5 Partition Coefficient

log Pow: 1.58 - 1.73
Method: OECD Guide-line 107 "Partition Coefficient (n-octanol/water), Flask-shaking Method"
Year:
Source: Phenolchemie GmbH Gladbeck

(9)

log Pow: 1.58 - 1.8
Method: other (measured)
Year:
GLP: no data
Remark: compilation of literature data
Source: Phenolchemie GmbH Gladbeck

(10)

log Pow: 1.58
Method: other (calculated)
Year:
Source: Phenolchemie GmbH Gladbeck

(11)

log Pow: 1.63 - 1.65
Method: other (measured)
Year:
GLP: no data
Source: Phenolchemie GmbH Gladbeck

(12)

2.6.1 Water Solubility

Value: 5.5 g/l at 20 degree C
Method: other
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(13)

Value: 8 g/l at 20 degree C
Method: other
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(6)

Value: 6.1 g/l at 25 degree C
Method: other: batch test under equilibrium conditions; testing period: 72h; determination of substance concentration by HPLC
Source: Phenolchemie GmbH Gladbeck
(14)

Value: 5.44 g/l
Method: other
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(15)

Value: 5.88 g/l
Method: other
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(16) (17)

2.6.2 Surface Tension

-

2.7 Flash Point

Value: 82 degree C
Type:
Method: other
Year:
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(18)

Value: 82.2 degree C
Type: open cup
Method: other
Year:
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(5)

Value: 105 degree C
Type: closed cup
Method: other
Year:
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(19)

Value:
Type: open cup
Method: other: DIN 51758
Year:
GLP: no data
Remark: range: 81–83 degree C
Source: Phenolchemie GmbH Gladbeck
(20)

2.8 Auto Flammability

Value: 535 degree C at 1013 hPa
Method: other
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(21)

Value: 571 degree C at 1013 hPa
Method: other
GLP: no data
Source: Phenolchemie GmbH Gladbeck
(22)

2.9 Flammability

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2.10 Explosive Properties

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2.11 Oxidizing Properties

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2.12 Additional Remarks

Remark: Odour threshold (air): 0.3 ppm (absolut; recognition at 0.6 ppm); pleasant sweet almond odour
Source: Phenolchemie GmbH Gladbeck
(23)

Remark: Odour threshold (water): 0.052 mg/l
Source: Phenolchemie GmbH Gladbeck
(24)

Remark: Odour threshold (air) : 1.5 mg/m3
(water): 65.0 mg/l
Source: Phenolchemie GmbH Gladbeck

(25)

3.1.1 Photodegradation

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3.1.2 Stability in Water

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3.1.3 Stability in Soil

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3.2 Monitoring Data (Environment)

Type of measurement: background concentration
Medium: air
Remark: Sample: urban air/Belgium
Result: identified in aerosol but not quantified
Source: Phenolchemie GmbH Gladbeck
(26)

Type of measurement: background concentration
Medium: air
Remark: Location: forest, Eggegebirge/Germany
Result: identified but not quantified; source unknown
Source: Phenolchemie GmbH Gladbeck
(27)

Type of measurement: background concentration
Medium: air
Remark: Location: Black Forest/Germany
Result: identified but not quantified
Source: Phenolchemie GmbH Gladbeck
(28)

Type of measurement: background concentration
Medium: drinking water
Remark: samples from 10 US cities; found in 1 sample
Result: concentration: 1 ug/l
Source: Phenolchemie GmbH Gladbeck
(29)

Type of measurement: background concentration
Medium: other: mother’s milk
Remark: Location: 4 urban areas in the USA
Result: substance was found in 8 from 12 samples but not quantified
Source: Phenolchemie GmbH Gladbeck
(30)

Type of measurement: background concentration
Medium: biota
Remark: determination of flavor volatiles of different cultivars of apricot
Result: concentration range: 11–488 ug/kg
Source: Phenolchemie GmbH Gladbeck
(31)

Type of measurement: background concentration
Medium: drinking water
Remark: Tap water from Kitakyushu/Japan
Result: concentration: 5.4 ug/l
Source: Phenolchemie GmbH Gladbeck
(32)

Type of measurement: background concentration
Medium: air
Remark: Location: 35 urban, rural or source dominated outdoor sites in the USA
date: from 1980 to 1985
Result: average: 0.722 ppbv
Source: Phenolchemie GmbH Gladbeck
(33)

Type of measurement: background concentration
Medium: other: volatiles of European bird cherry flowers (Padius avium)
Result: concentration: < 0.1%
Source: Phenolchemie GmbH Gladbeck
(34)

Type of measurement: concentration at contaminated site
Medium: surface water
Remark: Location: Hamilton harbour, Bermuda
Result: identified but not quantified, possible photoxidation product of ethylbenzene
Source: Phenolchemie GmbH Gladbeck
(35)

Type of measurement: concentration at contaminated site
Medium: other: secondary effluent from municipal wastewater treatment plants
Remark: Location: 8 wastewater treatment plants, Illinois/USA
Result: identified in the effluent of 2 of the plants but not quantified
Source: Phenolchemie GmbH Gladbeck
(36)

Type of measurement: concentration at contaminated site
Medium: sediment
Remark: Location: 4 inshore industrial sites at the Great Lakes/USA
Result: 2 ug/g dry weight at 1 of the sites, not detected at the other sites and 1 unpolluted reference site (detection limit: 0.02–0.39 ug/g)
Source: Phenolchemie GmbH Gladbeck
(37)

Type of measurement: concentration at contaminated site
Medium: air
Remark: Compilation of literature data concerning the airborne emissions of livestock buildings
Result: Substance was identified in the air of pig houses by several authors but not quantified.
Source: Phenolchemie GmbH Gladbeck
(38)

Type of measurement: concentration at contaminated site
Medium: other: percolate of a sanitary landfill
Remark: Location: Nordwijk/NL
date: 1979
no information concerning the source
Result: range: < 0.1–10 ug/l (dependent on soil depth)
Source: Phenolchemie GmbH Gladbeck
(39)

Type of measurement: other
Medium: surface water
Remark: Location: Bormida–Alessandria, Piedmont/Italy
date: 3/1990
no information concerning the source
Result: concentration: 1390 ug/l
Source: Phenolchemie GmbH Gladbeck
(40)

3.3.1 Transport between Environmental Compartments

Type: adsorption
Media: water – soil
Method: other: calculated on basis of molecular connectivity indices
Year:
Result: Soil sorption coefficient Koc: 79.4
Source: Phenolchemie GmbH Gladbeck
(41)

Type: adsorption
Media: water – soil
Method: other: measured
Year:
Result: Soil sorption coefficient Koc: 42.7
Source: Phenolchemie GmbH Gladbeck
(42)

Type: adsorption
Media: water – soil
Method: other: compilation of literature data
Year:
Result: Average soil sorption coefficient Koc (from 30 references): 43
Source: Phenolchemie GmbH Gladbeck
(43)

Type: adsorption
Media: water – soil
Method: other: determination of adsorption isotherms with 13 agricultural israelian soils and 4 recent israelian lake sediments by a batch method with 5 initial concentrations each
Year:
Result: Sorption coefficients Koc: 8.9–82.4 (soils with organic matter content between 0.17 and 5.82%; average: 24.5); 14.0–23.7 (sediments with organic matter content between 3.08 and 7.85%; average: 16.8)
soil sorption coefficients decreased with increasing organic matter content
Source: Phenolchemie GmbH Gladbeck
(44)

Type: adsorption
Media: water – soil
Method: other: RP–HPLC (cyanopropyl– and octadecylsilane column) with different mobile phases; correlation of capacity factors
Year:
Result: Soil sorption coefficient Koc: 53.7
Source: Phenolchemie GmbH Gladbeck
(45)

Type: adsorption
Media: water – soil
Method: other: batch tests with 3 soils of different content of organic carbon (0.05; 0.11; 1.2% dry weight); initial substance concentration: 0.5–1.0 mg/l; exposure time: 24 h; determination of final substance concentration by HPLC.
Year:
Remark: Koc decreased with increasing content of organic carbon.
Result: Soil sorption coefficients Koc: 270+/–80; 185+/–8; 105+/–4
Source: Phenolchemie GmbH Gladbeck
(14)

3.3.2 Distribution

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3.4 Mode of Degradation in Actual Use

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3.5 Biodegradation

Type: aerobic
Inoculum: activated sludge, industrial
Degradation: 94 % after 6 day
Method: OECD Guide–line 302 B "Inherent biodegradability: Modified Zahn–Wellens Test"
Year: **GLP:** no data
Test substance: no data
Remark: elimination by abiotic processes: 22%
no acclimation phase observed
Source: Phenolchemie GmbH Gladbeck
Test condition: substance concentration: 50–400 mg/l related to DOC

(46)

Type: aerobic
Inoculum: other: river water (Ohio river/USA)
Concentration: 20.5 mg/l related to Test substance
Degradation: 50 % after 6 day
Method: other: determination of carbon dioxide production; temperature 22–25 degree C; pH 7.2+/–0.1; redosing after 10 d
Year: **GLP:**
Test substance:
Remark: lag phase of about 3 d after addition of the 1st dose; 50% degradation of the 2nd dose after 3 d due to acclimation of the microorganisms; negligible nitrification interference in the substrate.
Source: Phenolchemie GmbH Gladbeck

(47)

Type: aerobic
Inoculum: activated sludge
Concentration: 100 mg/l related to Test substance
Degradation: > 30 % after 14 day
Method: other: determination of total organic carbon; ratio test substance/activated sludge: 100 ppm/30ppm; temperature: 25+/–2 degree C; pH 7.0+/–1
Year: **GLP:**
Test substance:
Source: Phenolchemie GmbH Gladbeck

(48)

Type: aerobic
Inoculum: other: (a) ground water; (b) river water; (c) water from harbour
Method: other: standard BOD technique by APHA (1980); test temperature: 21+/–3 degree C; substance concentrations: 0, 0.8, 1.6, 3.2 ul/l
Year: **GLP:** no data
Test substance:
Remark: (a) 39% of theoret. BOD after 20 d; rate constant: 0.022 d–1; t1/2: 32 d
(b) 70% of theoret. BOD after 15 d; rate constant: 0.083 d–1; t1/2: 8 d
(c) 75% of theoret. BOD after 15 d; rate constant: 0.155+/–0.025 d–1; t1/2: 4–4.5 d
biodegradation by first–order kinetics
Source: Phenolchemie GmbH Gladbeck
(49) (50)

3.6 BOD5, COD or BOD5/COD Ratio

Method: other: AFNOR NF T 90/103 (1969)

Result: BOD5: 32% of COD
Source: Phenolchemie GmbH Gladbeck
(51)

B O D 5

Method: other: standard dilution method, no further information
Year: **GLP:** no data
BOD5: 518 mgO2/l

Result: BOD10: 1.40 g/l
Source: Phenolchemie GmbH Gladbeck
(52)

3.7 Bioaccumulation

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3.8 Additional Remarks

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AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish

Type: flow through
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
LC50: 162
Method: other: bioassay in Lake Superior water; test temperature 24.6 degree C; pH 7.83; age/mean length of fish 31 d/15.7 mm
Year: **GLP:**
Test substance:
Remark: Affected fish lost equilibrium prior to death, fish at a nominal concentration of 148 mg/l did not school
Source: Phenolchemie GmbH Gladbeck
(53) (54)

Type: other: QSAR study
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mmol/l **Analytical monitoring:**
LC50: 2.4
Method: other: calculated
Year: **GLP:**
Test substance:
Source: Phenolchemie GmbH Gladbeck
(55)

Type: other: QSAR study
Species: Pimephales promelas (Fish, fresh water)
Exposure period:
Unit: g/l **Analytical monitoring:**
LC50: .162
Method: other: calculated
Year: **GLP:**
Test substance:
Source: Phenolchemie GmbH Gladbeck
(56)

Type: static
Species: Pimephales promelas (Fish, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** no
LC50: 155
Method: other: bioassay in Lake Superior water/USA; temperature: 18-22 degree C; fish size: 1.1-3.1 cm
Year: **GLP:** no data
Test substance: other TS
Remark:

Exposure time (h)	1	24	48	72	96
LC50 (mg/l)	>200	>200	163	158	155

Source: Phenolchemie GmbH Gladbeck
(57)

4.2 Acute Toxicity to Aquatic Invertebrates

-

4.3 Toxicity to Aquatic Plants e.g. Algae

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4.4 Toxicity to Microorganisms e.g. Bacteria

Type:
Species: other bacteria: mixed culture; isolated from wastewater samples by an enrichment culture technique
Exposure period: 75 minute(s)
Unit: mg/l **Analytical monitoring:** no
EC50: 1904
Method: other: biodegradation in a Warburg apparatus; test temperature: 30 degree C; correction for endogeneous respiration and abiotic oxidation
Year: **GLP:** no data
Test substance:
Remark: Result given as the chemical concentration that can reduce the maximum biodegradation rate of the substance by 50%.
Source: Phenolchemie GmbH Gladbeck

(58)

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish

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4.5.2 Chronic Toxicity to Aquatic Invertebrates

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TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Soil Dwelling Organisms

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4.6.2 Toxicity to Terrestrial Plants

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4.6.3 Toxicity to other Non–Mamm. Terrestrial Species

Species: Drosophila melanogaster (arthropod (Diptera))
Endpoint: mortality
Expos. period: 1 minute(s)
Unit: other: saturated atmosphere; gas concentration umol
LC50: 1.3
Method: other: test funnel presaturated with substance vapour; temperature 24 degree C
Year: **GLP:**
Test substance:
Source: Phenolchemie GmbH Gladbeck

(59)

4.7 Biological Effects Monitoring

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4.8 Biotransformation and Kinetics

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4.9 Additional Remarks

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5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 900 mg/kg bw
Method: other
Year: **GLP:**
Test substance: no data
Source: Phenolchemie GmbH Gladbeck

(60)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 3000 mg/kg bw
Method: other
Year: **GLP:**
Test substance: no data
Source: Phenolchemie GmbH Gladbeck

(61)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: = 2080 mg/kg bw
Method: other
Year: **GLP:**
Test substance: as prescribed by 1.1 – 1.4
Remark: original data: 2.02 ml/kg
Source: Phenolchemie GmbH Gladbeck

(62)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Value: = 740 mg/kg bw
Method: other
Year: **GLP:**
Test substance:
Source: Phenolchemie GmbH Gladbeck

(63)

5.1.2 Acute Inhalation Toxicity

Type: other: acute exposure
Species: rat
Sex:
Number of Animals:
Vehicle:
Exposure time: 8 hour(s)
Value:
Method: other
Year: **GLP:**
Test substance: no data
Remark: exposed to vapour saturated air for 8 h; no deaths observed
Source: Phenolchemie GmbH Gladbeck

(61)

5.1.3 Acute Dermal Toxicity

Type: other: dermal absorption
Species: mouse
Sex:
Number of Animals:
Vehicle:
Value:
Method: other: tails immersed in acetophenone for 4 h
Year: **GLP:**
Test substance:
Remark: all animals died
Source: Phenolchemie GmbH Gladbeck

(64)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: = 1760 mg/kg bw
Method: other
Year: **GLP:**
Test substance: no data
Source: Phenolchemie GmbH Gladbeck

(65)

Type: LD50
Species: rabbit
Sex:
Number of Animals:
Vehicle:
Value: = 15900 mg/kg bw
Method: other
Year: **GLP:**
Test substance:
Source: Phenolchemie GmbH Gladbeck

(66)

Type: LD50
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: > 20600 mg/kg bw
Method: other
Year: **GLP:**
Test substance: no data
Remark: original data: > 20 ml/kg
Source: Phenolchemie GmbH Gladbeck

(67)

5.1.4 Acute Toxicity, other Routes

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: = 200 mg/kg bw
Method: other
Year: **GLP:**
Test substance:
Source: Phenolchemie GmbH Gladbeck

(68)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Route of admin.: i.p.
Value: = 1070 mg/kg bw
Method: other
Year: **GLP:**
Test substance:
Remark: At doses of 400–500 mg/kg depression of the central nervous system was observed.
Source: Phenolchemie GmbH Gladbeck

(69)

Type: LDLo
Species: mouse
Sex:
Number of Animals:
Vehicle:
Route of admin.: s.c.
Value: = 330 mg/kg bw
Method: other
Year: **GLP:**
Test substance:
Source: Phenolchemie GmbH Gladbeck

(70)

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: slightly irritating
EC classificat.:
Method: other: FDA method, Code of Federal Regulations, Title 16, Section 1500.41 – 0.5 ml, 24 h, occlusive on normal and scarified skin; skin scoring according to Draize
Year: **GLP:** no
Test substance: as prescribed by 1.1 – 1.4
Remark: 4/6 rabbits with very slight oedema after 24 h on intact skin and 2/6 with very slight erythema; 5/6 with very slight oedema after 24 h on scarified skin, 3/6 with very slight erythema; after 72 h all reactions had normalized; irritation score: 0.63.
Source: Phenolchemie GmbH Gladbeck

(71)

Species: rabbit
Concentration:

Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: slightly irritating
EC classificat.:
Method: other: 24 h/occlusive
Year: **GLP:**
Test substance:
Remark: irritation described as mild burn
Source: Phenolchemie GmbH Gladbeck

(72)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: not irritating
EC classificat.:
Method: other: FDA method, Code of Federal Regulations, Title 16, Section 1500.42 – 0.1 ml were administered to the conjunctival sac; scoring after 24, 48 and 72 h according to Draize
Year: **GLP:** no
Test substance: as prescribed by 1.1 – 1.4
Remark: 6/6 rabbits without reactions due to test substance; irritation score: 0.
Source: Phenolchemie GmbH Gladbeck

(73)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: moderately irritating
EC classificat.:
Method: other: 771 mg pure acetophenone applied
Year: **GLP:**
Test substance:
Remark: moderate irritation and transient corneal injury
Source: Phenolchemie GmbH Gladbeck

(74)

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of Animals:
Result: irritating
EC classificat.:
Method: other: pure acetophenone or 2 drops of saturated aqueous solution tested
Year: **GLP:**
Test substance:
Remark: pure liquid: rather severe initial reaction: scored 8 on scale of 1-10;
2 drops: discomfort, eyes entirely normal within 30 min
Source: Phenolchemie GmbH Gladbeck

(75)

5.3 Sensitization

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5.4 Repeated Dose Toxicity

Species: rat **Sex:** male/female
Strain: other: Sherman
Route of admin.: oral feed
Exposure period: 30 days
Frequency of treatment: daily
Post. obs. period:
Doses: 1 (minimum) - 102 (maximum) mg/kg/day
Control Group: yes, concurrent vehicle
Method: other
Year: **GLP:**
Test substance: no data
Remark: 5 rats/sex/group
Result: Maximum dose without effect on growth, appetite and micropathology: > 102 mg/kg/day
Source: Phenolchemie GmbH Gladbeck

(60)

Species: rat **Sex:**
Strain:
Route of admin.: oral feed
Exposure period: 17 weeks
Frequency of treatment: daily
Post. obs. period: no data
Doses: 750 mg/kg/day
Control Group:
Method: other
Year: **GLP:**
Test substance:
Remark: original data: 10000 ppm in the diet; conversion according to Lehman, A.J. (1954), Assoc. Food Drug Off. Q. Bull. 18, 66
Result: no toxic effects observed
Source: Phenolchemie GmbH Gladbeck

(76)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium TA 98, TA 100, TA 1535, TA 1537
Concentration: 8-5000 ug/plate
Metabolic activation: with and without
Result: negative
Method: other
Year: **GLP:** no data
Test substance: other TS: > 99% purity
Source: Phenolchemie GmbH Gladbeck

(77)

Type: Cytogenetic assay
System of testing: Chinese hamster cells (CHL)
Concentration: 0-1.2 mg/ml
Metabolic activation: with
Result: positive
Method: other
Year: **GLP:** no data
Test substance: no data
Remark: chromosomal aberrations tested; without metabolic activation negative
Source: Phenolchemie GmbH Gladbeck

(78)

Type: DNA damage and repair assay
System of testing: DNA from bacteriophage PM2
Concentration: 2.7 M
Metabolic activation: without
Result: positive
Method: other: endonuclease-sensitive modifications and single strand breaks induced by UV (333 nm) irradiation were investigated in the presence and absence of acetophenone
Year: **GLP:** no data
Test substance: other TS
Remark: see also section 5.10 (Demidov et al., 1991)
Source: Phenolchemie GmbH Gladbeck
Test substance: purity: 99%

(79)

Type: DNA damage and repair assay
System of testing: Salmonella typhimurium TA 1535/pSK1002
Concentration: 680.3 ug/ml
Metabolic activation: with and without
Result: negative
Method: other: umu-test (umu operon is induced by DNA-damaging agents)
Year: 1985 **GLP:** no data
Test substance: no data
Source: Phenolchemie GmbH Gladbeck

(80)

5.6 Genetic Toxicity 'in Vivo'

-

5.7 Carcinogenicity

-

5.8 Toxicity to Reproduction

-

5.9 Developmental Toxicity/Teratogenicity

Species: rat **Sex:** female
Strain:
Route of admin.: dermal
Exposure period: day 10–15 of gestation
Frequency of treatment: once/day
Duration of test:
Doses: 480 mg/kg/day
Control Group:
Method:
Year: **GLP:**
Test substance:
Result: no changes in the gestation period, size of litter, weight of offspring, time for teeth and hair appearance, opening of the eyes or appearance of reflexes observed
Source: Phenolchemie GmbH Gladbeck

(64)

5.10 Other Relevant Information

Type: Metabolism
Remark: Within 1–3 days a total dose of 100 mg/kg was administered i.p. to Albino rats (8 m). Urine was collected up to 24 h after the final dose. Chemical analysis revealed mandelic acid (detection by optical activity) and benzoylformic acid as final metabolites (other intermediates: omega–hydroxyacetophenone (o–HA), phenylglyoxal or phenylethylene glycol, and phenylglycol aldehyde. – The reaction of acetophenone to o–HA was found to be mediated by rat and rabbit liver microsomes in vitro and in rabbit also in vivo. – Conversion of acetophenone to benzoic acid was found, too. Using (methyl–C–14)–acetophenone (100 mg/kg,i.p., rat) 10% of the radioactivity were exhaled as CO2 within 4 h and 30% within 13 h.
Source: Phenolchemie GmbH Gladbeck
Test substance: boiling point: 200–202 degrees C

(81)

Type: Metabolism
Remark: Acetophenone was converted to methyl phenylcarbonal and benzoic acid. The benzoic acid was conjugated with glycine and excreted in the urine as hippuric acid.
Source: Phenolchemie GmbH Gladbeck

(82)

Type: Metabolism
Remark: Acetophenone is largely metabolized to benzoic acid (91.7%) appearing in the urine as hippuric acid.
Source: Phenolchemie GmbH Gladbeck
Test substance: no data

(83)

Type: other: DNA-photosensitizing activity (PSA)
Remark: The DNA fragment desoxythymidine-mono(or di-)nucleotide was used to test acetophenone for DNA-photosensitizing activity (PSA). Water solutions of the nucleotide were irradiated with UV (310-390 nm) in the presence or absence of acetophenone (2 mM). The formation of cyclobutane dimers was detected by HPLC (vehicle control: 1-4%; acetophenone: 15-38%).
Source: Phenolchemie GmbH Gladbeck

(84)

Type: other: sensory irritation test
Remark: A sensory irritation test based on trigeminal nerve stimulation in the nasal mucosa of rodents resulted in a decreased respiratory frequency. For acetophenon an RD50-value (= 50% decrease in the respiratory rate) of 0.5 mg/l (= 100 ppm) was reported for Swiss OF1 mice after 5-15 min of exposure.
Source: Phenolchemie GmbH Gladbeck

(85)

5.11 Experience with Human Exposure

Remark: 6-month study with 9 volounteers (New York, USA): acetophenone was detected in 5 of 12 breath samples (personal sampling); analysis of air and drinking water: acetophenone was identified in 4 of 8 air samples and in one drinking water sample; no quantification; no information concerning the source; detection limits: 1ug/m3 (air, breath); 1ng/l (water).
Source: Phenolchemie GmbH Gladbeck

(86)

Remark: Inhalation of 0.4 mg/l (= 80 ppm) for 60 min caused a severe intoxication; no further information available.
Source: Phenolchemie GmbH Gladbeck
Test substance: no data

(87)

Remark: No skin sensitization was observed after administration of 2% acetophenone in petrolatum.
Source: Phenolchemie GmbH Gladbeck

(88)

Remark: Among healthy subjects no effects were observed after ingestion of 100-300 mg; with 450-600 mg micturition was increased, pulse weakened and slowed after 5-6 h, and slight but continuous decrease of haemoglobin was observed (reversible)
Source: Phenolchemie GmbH Gladbeck

(89)

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7.1 Risk Assessment

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