

I U C L I D

D a t a s e t

Existing Chemical	Substance ID: 20306-75-6
CAS No.	20306-75-6
EINECS Name	N-methyl-3-oxobutyramide
EINECS No.	243-723-9
Molecular Formula	C5H9NO2

Dataset created by: EUROPEAN COMMISSION - European Chemicals Bureau

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

Creation date: 18-FEB-2000

Number of Pages: 17

Chapters: all

Edition: Year 2000 CD-ROM edition

Flags: non-confidential

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1.0.1 OECD and Company Information

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1.0.2 Location of Production Site

-

1.0.3 Identity of Recipients

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1.1 General Substance Information

Substance type: organic
Physical status: liquid

Substance type: organic
Physical status: solid

1.1.1 Spectra

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1.2 Synonyms

2-Acetyl-N-methylacetamide
Source: LONZA AG Basel

acetic acid, N-methylamide
Source: Wacker - Chemie GmbH Burghausen

Butanamide, N-methyl-3-oxo- (9CI)
Source: LONZA AG Basel

N-methyl-3-oxobutanamide
Source: Wacker - Chemie GmbH Burghausen

N-methyl-3-oxobutyramide
Source: Wacker - Chemie GmbH Burghausen

N-Methylacetessigsäureamid
Source: LONZA AG Basel

N-Methylacetoacetamide
Source: LONZA AG Basel

1.3 Impurities

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1.4 Additives

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1.5 Quantity

Quantity 5 000 - 10 000 tonnes

1.6.1 Labelling

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1.6.2 Classification

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1.7 Use Pattern

Type: type
Category: Non dispersive use

Type: type
Category: Use in closed system

Type: industrial
Category: Chemical industry: used in synthesis

Type: industrial
Category: Textile processing industry

Type: use
Category: Colouring agents

Type: use
Category: Intermediates

Type: use
Category: Pesticides

1.7.1 Technology Production/Use

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1.8 Occupational Exposure Limit Values

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1.9 Source of Exposure

Remark: Herstellung erfolgt in einer emissionsfreien Anlage, deren Abluft zentral verbrannt wird.
Source: Wacker - Chemie GmbH Burghausen

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: = -3 degree C
Method: other
GLP: no data
Source: Wacker - Chemie GmbH Burghausen (1)

2.2 Boiling Point

Value: = 118 degree C at 6.7 hPa
Method: other
GLP: no data
Source: Wacker - Chemie GmbH Burghausen (1)

2.3 Density

Type: relative density
Value: = 1.087 g/cm³ at 15.6 degree C
Method: other
GLP: no data
Remark: relative to the density of water at 15.55 degree C.
Source: Wacker - Chemie GmbH Burghausen
Test substance: 70% aqueous solution (2)

Type: density
Value: = 1.06 - 1.07 g/cm³ at 20 degree C
Method: other
GLP: no data
Source: Wacker - Chemie GmbH Burghausen
Test substance: 50-70% aqueous solution. (3)

Type: relative density
Value: = 1.1 g/cm³ at 20 degree C
Method: other
GLP: no data
Source: Wacker - Chemie GmbH Burghausen
Test condition: relative to the density of water at 4 degree C. (1)

2.3.1 Granulometry

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2.4 Vapour Pressure

Value: = 20 hPa at 20 degree C
Method: other (measured)
GLP: no data
Source: Wacker - Chemie GmbH Burghausen (1)

2.5 Partition Coefficient

log Pow: = -1.046
Method:
Year:
GLP: no data
Remark: octanol/water partition coefficient 0.09+/-0.03
Source: Wacker - Chemie GmbH Burghausen (1)

2.6.1 Water Solubility

Method: other
GLP: no data
Remark: solubility in water: complete.
Source: Wacker - Chemie GmbH Burghausen
Test substance: 70% aqueous solution (2)

2.6.2 Surface Tension

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2.7 Flash Point

Value: = 101 degree C
Type: closed cup
Method: other
Year:
GLP: no data
Source: Wacker - Chemie GmbH Burghausen
Test substance: 50-70% aqueous solution. (3)

Value: = 105 degree C
Type: other
Method: other
Year:
GLP: no data
Remark: no data about type.
Source: Wacker - Chemie GmbH Burghausen (1)

2.8 Auto Flammability

Value: = 349 degree C
Method: other
GLP: no data
Remark: method: ASTM D 2155
Source: Wacker - Chemie GmbH Burghausen
Test substance: 70% aqueous solution (2)

Value: = 458 degree C
Method: other
GLP: no data
Source: Wacker - Chemie GmbH Burghausen (1)

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: TS stable, no hazardous polymerisation; oxidizing materials can cause a reaction.
Source: Wacker - Chemie GmbH Burghausen
Test substance: 70% aqueous solution (2)

Remark: conversion factor 1 mg/m³ = 0.21 ppm
Source: Wacker - Chemie GmbH Burghausen (1)

Remark: vapor density (air = 1) ca. 4.
Source: Wacker - Chemie GmbH Burghausen (1)

Remark: soluble in polar organic solvents, not very soluble in unpolar org. solvents.
Source: Wacker - Chemie GmbH Burghausen (1)

Remark: lower explosive limit 1.8 Vol.%
Source: Wacker - Chemie GmbH Burghausen (1)

Remark: method: the thermal conductivity of the a) aqueous TS solution (48% water) at 25 degree C and b) 90% TS in toluene at 50 degree C was measured.
result: a) 220.0 and b) 148.8 E-5 J/cm/S/degree C.

Source: Wacker - Chemie GmbH Burghausen

(4)

Remark: strong fish-like odor

Source: Wacker - Chemie GmbH Burghausen

(2)

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)

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3.3.1 Transport between Environmental Compartments

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3.3.2 Distribution

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3.4 Mode of Degradation in Actual Use

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3.5 Biodegradation

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3.6 BOD5, COD or BOD5/COD Ratio

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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: semistatic
Species: Salmo gairdneri (Fish, estuary, fresh water)
Exposure period: 96 hour(s)
Unit: mg/l **Analytical monitoring:** yes
LC50: > 1000
Method: Directive 84/449/EEC, C.1 "Acute toxicity for fish"
Year: 1984 **GLP:** yes
Test substance: other TS
Remark: method: daily renewal of media, verified by chemical analysis at 0, 24 and 96 h.
result: no adverse effects in any fish throughout the study.
Source: Wacker - Chemie GmbH Burghausen
Test condition: dechlorinated tap water; total hardness 350 mg/l CaCO₃; one test concentration: 1000 mg/l (equivalent to 700 mg a.i./l); 1 replicate; 10 fishes per group; temperature 13.0 degree C; pH 7.8-8.0; 10.2-10.5 mg O₂ per l.
Test substance: 70% aqueous solution

(5)

4.2 Acute Toxicity to Aquatic Invertebrates

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4.3 Toxicity to Aquatic Plants e.g. Algae

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4.4 Toxicity to Microorganisms e.g. Bacteria

Type: aquatic
Species: activated sludge of a predominantly domestic sewage
Exposure period: 30 minute(s)
Unit: mg/l **Analytical monitoring:** no data
EC50: > 16000
Method: Directive 87/302/EEC, part C, p. 118 "Biodegradation: Activated sludge respiration inhibition test"
Year: 1987 **GLP:** yes
Test substance: other TS
Remark: method: respiration inhibition test after a) 30 min or b) 3 h contact time.
result: b) EC50 > 16000 mg/l; 15% increased oxygen consumption in a), no inhibition in b) compared to control value.
Source: Wacker - Chemie GmbH Burghausen
Test condition: continuous aeration; temperature 23 degree C; TS concentration in a) and b) 16000 mg/l (equivalent to 11200 mg a.i./l); duplicate test.
Test substance: 70% aqueous solution

(6)

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

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4.7 Biological Effects Monitoring

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4.8 Biotransformation and Kinetics

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4.9 Additional Remarks

Remark: method: maize, cabbage and apple were treated with the C14 labelled insecticide monocrotophos and the breakdown products were studied.

Source: result: TS was one of the breakdown products.
Wacker - Chemie GmbH Burghausen

(7)

Remark: method: products and rates of hydrolysis and soil metabolism of the insecticide monocrotophos were studied.

Source: result: the TS was degradation product in both.
Wacker - Chemie GmbH Burghausen

(8)

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: > 3200 mg/kg bw
Method: other
Year: **GLP:** no data
Test substance: other TS
Remark: validity: no further information available.
Source: Wacker - Chemie GmbH Burghausen
Test substance: 70% aqueous solution

(2)

Type: LD50
Species: rat
Sex:
Number of Animals:
Vehicle:
Value: > 5000 mg/kg bw
Method: other
Year: **GLP:** no data
Test substance: other TS
Remark: validity: no further information available.
Source: Wacker - Chemie GmbH Burghausen
Test substance: 10% aqueous solution

(3)

Type: LD50
Species: mouse
Sex:
Number of Animals:
Vehicle:
Value: > 3200 mg/kg bw
Method: other
Year: **GLP:** no data
Test substance: other TS
Remark: validity: no further information available.
Source: Wacker - Chemie GmbH Burghausen
Test substance: 70% aqueous solution

(2)

5.1.2 Acute Inhalation Toxicity

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5.1.3 Acute Dermal Toxicity

Type: LD50
Species: guinea pig
Sex:
Number of Animals:
Vehicle:
Value: > 1000 mg/kg bw
Method: other
Year: **GLP:** no data
Test substance: other TS
Remark: method: tested with anhydrous material.
validity: no further information available.
Source: Wacker - Chemie GmbH Burghausen
Test substance: see method

(2)

5.1.4 Acute Toxicity, other Routes

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5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: guinea pig
Concentration:
Exposure:
Exposure Time:
Number of Animals:
PDII:
Result: slightly irritating
EC classificat.:
Method: other
Year: **GLP:** no data
Test substance: other TS
Remark: result: repeated application led to slight exacerbation.
validity: no further information available.
Source: Wacker - Chemie GmbH Burghausen
Test substance: 70% aqueous solution

(2)

5.2.2 Eye Irritation

Species: rabbit
Concentration:
Dose:
Exposure Time:
Comment:
Number of
Animals:
Result: slightly irritating
EC classificat.:
Method: other
Year: GLP: no data
Test substance: other TS
Remark: validity: no further information available.
Source: Wacker - Chemie GmbH Burghausen
Test substance: 70% aqueous solution

(2)

5.3 Sensitization

Type: other
Species: guinea pig
Number of
Animals:
Vehicle:
Result:
Classification:
Method: other
Year: GLP: no data
Test substance: other TS
Remark: result: slight sensitization of the skin.
validity: no further information available.
Source: Wacker - Chemie GmbH Burghausen
Test substance: 70% aqueous solution

(2)

5.4 Repeated Dose Toxicity

Species: rat **Sex:** no data
Strain: no data
Route of admin.: oral feed
Exposure period: 10 days
Frequency of treatment: no data
Post. obs. period: no data
Doses: 0.1 or 1% TS in the diet= ca. 90 or 940 mg/kg/d (63 or 658 mg/kg/d solute, respectively)
Control Group: no data specified
NOAEL: = 90 mg/kg bw
Method: other **GLP:** no data
Year:
Test substance: other TS
Remark: method: measured parameters: food intake, body weight; clinical signs, hematology, clinical chemistry, organ weights, macro- and microscopical pathology. validity: no further information available.
Result: at 1% relative liver weight and relative and absolute kidney weights slightly increased; no further effects.
Source: Wacker - Chemie GmbH Burghausen
Test substance: 70% aqueous solution

(2)

5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium TA 98, 100, 1535, 1537, 1538
Concentration: 2-200 microliter/plate
Metabolic activation: with and without
Result: negative
Method: other **GLP:** no data
Year:
Test substance: no data
Remark: method: incubation with the TS for 48 h at 37 degree C.
Source: Wacker - Chemie GmbH Burghausen

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5.6 Genetic Toxicity 'in Vivo'

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5.7 Carcinogenicity

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5.8 Toxicity to Reproduction

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5.9 Developmental Toxicity/Teratogenicity

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5.10 Other Relevant Information

Type: other
Remark: Teratogenicity in hen eggs
method: 30 hen eggs were injected with 1 mg TS into the yolk
on day 4 of incubation and teratogenic signs, body weight
and length determined on day 21.
result: 15 survivors, but no effects on survivors.
validity: no statistical evaluation.
Source: Wacker - Chemie GmbH Burghausen

(10)

5.11 Experience with Human Exposure

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7.1 Risk Assessment

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