I. General Information

201-14993

CAS Number: 2044-64-6
Name: Butanamide, N,N-dimethyl-3-oxo-
N,N-Dimethyl-3-oxobutyramide
Dimethylacetoacetamide
Acetoacetamide, n,n-dimethyl-
N,N-Dimethyl-3-oxobutanamide
N,N-Dimethylacetoacetamide

II. Physical-Chemical Data

A. Melting Point

Test Substance	
Test substance:	N,N-Dimethylacetoacetamide
Remarks:	
Method	
Method:	Estimation
Remarks:	Mean of the Joback, and the Gold and Ogle methods
Results	
Melting point value:	32 °C
Remarks:	
References	MPBPWIN v1.40 in EPIWIN v3.10, Syracuse Research Corporation, Syracuse, New York
Other	

B. Boiling Point

Test Substance	
Test substance:	N,N-Dimethylacetoacetamide
Remarks:	
Method	
Method:	Estimation
Remarks:	Adapted Steinand Brown method
Results	
Boiling point value:	220 °C
Remarks:	
References	MPBPWIN v1.40 in EPIWIN v3.10, Syracuse Research Corporation, Syracuse, New York
Other	

C. Vapor Pressure

Test Substance	
Test substance:	N,N-Dimethylacetoacetamide
Remarks:	
Method	
Method:	Estimation
Remarks:	Modified Grain method
Results	
Vapor pressure value:	0.105 mmHg
Temperature:	25 °C
Remarks:	
References	MPBPWIN v1.40 in EPIWIN v3.10, Syracuse Research Corporation, Syracuse, New York
Other	

D. Partition Coefficient

Test Substance	
Test substance:	N,N-Dimethylacetoacetamide
Remarks:	
Method	
Method:	Estimation
Remarks:	
Results	
Log K_{OW}:	-0.58
Remarks:	
References	KOWIN v1.66 in EPIWIN v3.10, Syracuse Research Corporation, Syracuse, New York
Other	

E. Water Solubility

Test Substance	
Test substance:	N,N-Dimethylacetoacetamide
Remarks:	
Method	
Method:	Estimation
Remarks:	
Results	
Value:	288.1 g/L
Temperature:	25 °C
Description:	Appreciable (100-999 g/L)
Remarks:	
References	WSKOW v1.40 in EPIWIN v3.10, Syracuse Research Corporation, Syracuse, New York
Other	

III. Environmental Fate Endpoints

A. Photodegradation

Test Substance	
Test substance:	N,N-Dimethylacetoacetamide
Remarks:	
Method	
Method:	Estimation
Test type:	Atmospheric oxidation
Remarks:	
Results	
Temperature:	25 °C
Hydroxyl radicals reaction	
OH Rate constant:	16.7426 x 10^{-12} cm^3/molecule-sec
Half-life	0.639 Days (12-hr day; 1.5x10^6 OH/cm^3)
Ozone reaction:	No ozone reaction estimation
Remarks:	
Conclusions	Material is oxidized by hydroxyl radicals in the atmosphere at a rapid rate.
References	AopWin v1.90 in EPIWIN v3.10, Syracuse Research Corporation, Syracuse, New York
Other	

C. Biodegradation

Test Substance	
Test substance:	N,N-dimethylacetoacetamide
Remarks:	Purity was 99.1% (area) by GC/FID, structure confirmed by GC/MS
Method	
Method:	Method C.9., "Degradation, Chemical Oxygen Demand", Official Journal of the European Communities, No. L251/214, 19.9.84
Test type:	Chemical Oxygen Demand (COD)
GLP:	Yes
Year:	1996
Remarks:	
Results	
Results:	0.791 grams COD/gram of test substance
Remarks:	The value is a mean of three replicates.
Conclusions	
Data Quality	
Remarks:	This was a well-documented study that followed established guidelines and was conducted under GLP assurances.
References	Chemical Oxygen Demand of Eastman DMAA; Chemicals Quality Services Division, Eastman Kodak Company, Rochester, NY; HAEL No. 96-0201, April 17, 1996.
Other	

Test Substance	
Test substance:	N,N-dimethylacetoacetamide
Remarks:	Purity was 99.1% (area) by GC/FID, structure confirmed by GC/MS
Method	
Method:	Method C.8., "Degradation, Biochemical Oxygen Demand", Official Journal of the European Communities, No. L251/212, 19.9.84.
Test type:	Biochemical Oxygen Demand (BOD)
GLP:	Yes
Year:	1996
Remarks:	BOD was determined after 5 and 20 days.
Results	
Results:	BOD5 was 0.0069 grams BOD/gram of test substance at 0.020, 0.030, 0.060 percent concentrations BOD20 was 0.011 grams BOD/gram of test substance at 0.020 and 0.030 percent concentrations
Remarks:	QC requirements conformed with method requirements
Conclusions	The test material is not considered to be "Readily Biodegradable" based on a BOD5/COD ratio greater less than 0.5 (0.0069/0.791=0.0087)
Data Quality	
Remarks:	This was a well-documented study that followed established guidelines and was conducted under GLP assurances.
References	Biochemical Oxygen Demand of Eastman DMAA; Chemicals Quality Services Division, Eastman Kodak Company, Rochester, NY; HAEL No. 96-0201, April 17, 1996.
Other	

D. Transport between Environmental Compartments (Fugacity)

Test Substance	
Test substance:	N,N-Dimethylacetoacetamide
Remarks:	
Method	
Test type:	Estimation
Model used:	Level III Fugacity Model; EPIWIN:EQC from Syracuse Research Corporation
Remarks:	
Results	
Model data and results:	Distribution (%)
Estimated distribution	Air 0.00118
and media concentration	Water 45.2
(levels II/III):	Soil 54.7
	Sediment 0.0755
Remarks:	Since no experimental values were available the physical chemical values utilized in this model were default parameters from within EPIWIN.
Conclusions	
References	Meylan, W. (1993). User's Guide for the Estimation Programs Interface (EPI), Version 3.10, Syracuse Research Corporation, Syracuse, New York 13210. The Level III model incorporated into EPIWIN is a Syracuse Research Corporation adaptation of the methodology described by Mackay *et al.* 1996; *Environ. Toxicol. Chem.* **15(9)**, 1618-1626 and 1627-1637.
Other	

IV. Ecotoxicity

A. Acute Toxicity to Fish

Test Substance	
Test substance:	N,N-dimethylacetoacetamide
Remarks:	Purity was 99.1% (area) by GC/FID, structure confirmed by GC/MS
Method	
Method:	OECD 203 and EEC/Annex V C.1.
Test type:	Static
GLP:	Yes
Year:	1997
Species/strain:	Fathead minnow (*Pimephales promelas*)
Analytical monitoring:	Yes; Exposure solutions, temperature, pH, dissolved oxygen
Exposure period:	96-Hour
Remarks:	Juvenile fish of <90 days in age were utilized. Biological loading was kept below 1.0 g wet weight per liter of test solution, with 14 fish used per exposure level (2 replicates of 7 fish).
Results	
Nominal concentration:	1000 mg/L
Measured concentration:	977.74 mg/L
Endpoint value:	96-hour LC_{50} >977.74 mg/L, 96-hour NOEC=977.74 mg/L
Biological observations:	No mortality was observed throughout the 96-hour exposure in the control or test substance
Statistical methods:	NA - No mortality was observed
Remarks:	The tests were performed in glass chromatography jars containing 20 L of exposure solution. Exposure temperature ranged from 19-20 °C, pH ranged from7.6 to 8.3, and dissolved oxygen ranged from 6.1 to 8.9 mg/L. The analyzed mean percent loss of the test substance ranged from 12.7% to 19.5%.
Conclusions	The 96-hour LC_{50} value indicates that the test substance would not be classified according to the European Union's labeling directive and would correspond to a "low concern level" according to the U.S. EPA's assessment criteria.
Data Quality	
Reliability:	Reliable without restrictions
Remarks:	This was a well-documented OECD guideline study conducted under GLP assurances.
References	An Acute Aquatic Effects Test with the Fathead Minnow (*Pimephales promelas*); Environmental Sciences Section, Health and Environment Laboratories, at Eastman Kodak Company, Rochester, NY; Study No. EN-430-909497-A; July 10, 1997.
Other	

B. Acute Toxicity to Aquatic Invertebrates

Test Substance	
Test substance:	N,N-dimethylacetoacetamide
Remarks:	Purity was 99.1% (area) by GC/FID, structure confirmed by GC/MS
Method	
Method:	OECD 202 and EEC/Annex V C.2.
Test type:	Acute immobilization, Static
GLP:	Yes
Year:	1997
Species/strain:	Daphnid (*Daphnia magna*)
Analytical monitoring:	Yes; Exposure solutions, temperature, pH, dissolved oxygen
Exposure period:	48-Hour
Remarks:	The study was conducted in general agreement with OECD test guideline 202 and European Community Annex V, Part C.2.
Results	
Nominal concentration:	1,000 mg/L
Measured concentration:	1,005 mg/L
Endpoint value:	48-hour EC_{50} >1005 mg/L, 48-hour NOEC=1,005 mg/L
Biological observations:	The daphnids in the dilution water controls and test substance exposure solutions exhibited normal behavior and appearance throughout the test and no mortality was observed during the study.
Statistical methods:	NA; No significant differences in immobility were noted between treated and controls.
Remarks:	The test substance exposure concentration was based on the arithmetic average (for replicates A and B) of the geometric means of the test substance analytical results at exposure start (time 0) and the test substance analytical results at exposure end (48-hours). Exposure temperature ranged from 20-21 °C, pH ranged from 8.2 to 8.3, and dissolved oxygen ranged from 8.2 to 8.9 mg/L. The analyzed mean percent gain of the test substance ranged from 21.5% to 24.0%.
Conclusions	The EC_{50} value indicates that the test substance would not be classified according to the European Union's labeling directive and would correspond to a "low concern level" according to the U.S. EPA's assessment criteria.
Data Quality	
Reliability:	Reliable without restrictions
Remarks:	This was a well-documented OECD guideline study conducted under GLP assurances.
References	An Acute Aquatic Effects Limit Test with the Daphnid (*Daphnia magna*); Environmental Sciences Section, Health and Environment Laboratories, at Eastman Kodak Company, Rochester, NY; Study No. EN-431-909497-A, September 18, 1997
Other	

V. Toxicological Data

A. Acute Toxicity

Test Substance	
Test substance:	N,N-Dimethylacetoacetamide
Remarks:	Purity was unknown
Method	
Method:	Acute lethality; Other
Test type:	LD_{50} estimate
GLP:	No (Pre-GLP)
Year:	1962
Species/strain:	Rat/unknown
Route of exposure:	Oral gavage
Dose levels:	200, 400, 800, 1,600 and 3,200 mg/kg
Remarks:	The report indicated that there were 10 animals used. It is assumed there were 2 rats/dose level administered.
Results	
Value:	LD_{50} = >3,200 mg/kg.
Deaths at each dose:	No mortalities were noted.
Remarks:	Animals were noted as appearing quite weak with vasodilatation. A gain in weight was reported after the 2-week study observation period was complete.
Conclusions	Material would be considered as slightly toxic.
Data Quality	
Reliability:	Reliable with restrictions
Remarks:	The study was conducted quite some time ago and hence many study details are missing from the report and not available. However, basic data are given and results indicate the material is not acutely toxic.
References	Toxicity Report, Laboratory of Industrial Medicine, Eastman Kodak Company, Rochester, NY. 9-14-62.
Other	

Test Substance	
Test substance:	N,N-Dimethylacetoacetamide
Remarks:	Purity was unknown
Method	
Method:	Acute lethality; Other
Test type:	LD_{50} estimate
GLP:	No (Pre-GLP)
Year:	1962
Species/strain:	Mouse/unknown
Route of exposure:	Oral gavage
Dose levels:	200, 400, 800, 1,600 and 3,200 mg/kg
Remarks:	The report indicated that there were 10 animals used. It is assumed there were 2 mice/dose level administered.
Results	
Value:	LD_{50} = >3,200 mg/kg.
Deaths at each dose:	No mortalities were noted.
Remarks:	Animals were noted as appearing slight to moderate weakness with a rough coat. A gain in weight was reported after the 2-week study observation period was complete.
Conclusions	Material would be considered as slightly toxic.
Data Quality	
Reliability:	Reliable with restrictions
Remarks:	The study was conducted quite some time ago and hence many study details are missing from the report and not available. However, basic data are given and results indicate the material is not acutely toxic.
References	Toxicity Report, Laboratory of Industrial Medicine, Eastman Kodak Company, Rochester, NY. 9-14-62.
Other	