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Fyrol 6

HPV Robust Summaries  
(Revised)

Submitted  
by  
Supresta

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## 1. Substance Information

<i>CAS Number:</i>	2781-11-5
<i>Chemical Name:</i>	Phosphonic acid, [[bis (2-hydroxyethyl) amino] methyl]-diethyl ester
<i>Structural Formula:</i>	C <sub>9</sub> H <sub>22</sub> NO <sub>5</sub> P
<i>Other Names:</i>	Diethyl [(diethanolamino) methyl] phosphonate; Fyrol 6
<i>Exposure Limits:</i>	None

## 2. Physical – Chemical Properties

### 2.1. Boiling Point:

Identity:	Fyrol 6; CAS# 2781-11-5; Batch 04106C0103; Purity 85%
Method:	OECD 103 and EPA OPPTS 830.7220
GLP:	Yes
Year:	2005
Value:	196°C
Conclusions:	The boiling point of Fyrol 6 was determined to be 196°C.
Reliability:	1
Reference:	1
Remarks:	None

### 2.2. Vapor Pressure:

Identity:	Fyrol 6; CAS# 2781-11-5; Lot 0106B-12; purity – 70-90%
Method:	OECD 104
GLP:	No
Year:	2000
Value:	0.43 mm Hg
Temperature° C:	20
Pressure Unit:	MmHg
Conclusions:	The vapor pressure of Fyrol 6 is C is 0.43 mmHg.
Reliability:	2
Reference:	2
Remarks:	Isoteniscope method

### **2.3. Partition Coefficient (log Kow):**

Identity:	Fyrol 6; CAS# 2781-11-5; Lot 0106B-12; purity – 70-90%
Method:	OECD 107
GLP:	No
Year:	2001
Log Kow:	-0.72
Temperature:	25 °C
Conclusions:	The log Kow of Fyrol 6 is -0.72
Reliability:	2
Reference:	3
Remarks:	None

### **2.4. Water Solubility:**

Identity:	Fyrol 6; CAS# 2781-11-5; Lot 0106B-12; purity – 70-90%
Method:	OECD 105
GLP:	No
Year:	2001
Solubility:	900 g/L at 25°C
Description:	Clear
pH value at 25 °C:	Not reported
pka value at 25°C:	Not reported
Conclusions:	The water solubility of Fyrol 6 is 900 g/L.
Reliability:	2
Reference:	4
Remarks:	Flask method

## **3. Environmental Fate**

### **3.1. Photodegradation:**

Identity:	Fyrol 6; CAS# 2781-11-5
Method:	EPIWIN Computer Model
GLP:	Not applicable
Type:	Not applicable
Year:	Not applicable
Light Source:	Not applicable
Light Spectrum (nm):	Not applicable
Half-life:	0.898 hours
Breakdown Products:	Not available
Conclusions:	The half-life in the atmosphere for Fyrol 6 is estimated to be 0.898 hours.
Reliability:	2
Reference:	5

### 3.2. Transport (Fugacity):

Identity:	Fyrol 6; CAS# 2781-11-5			
Method:	EPIWIN Computer Model			
GLP:	Not applicable			
Type:	Not applicable			
Year:	Not applicable			
Media:	Air, Water, Soil, Sediment			
Distributions:	Compartment	Released	Release 100%	Release 100%
		100% to air	to water	to soil
	Air	6.8	$3.98 \times 10^{-4}$	0.0213
	Water	35	99.8	31.8
	Soil	58.2	$3.4 \times 10^{-3}$	68.1
	Sediment	0.0645	0.184	0.0681
Conclusions:	Fyrol 6 is distributed primarily to water and soil.			
Reliability:	2			
Reference:	6			
Remarks:	When released equally to air, water and soil, Fyrol 6 is distributed 0.2% to air, 58.3% to water, 41.4% to soil and 0.1% to sediment.			

### 3.3. Stability in Water (Hydrolysis)

Identity:	Fyrol 6; CAS# 2781-11-5; Batch 04106C0103; Purity 85%
Method:	OECD 111 and EPA OPPTS 835.2110
Type:	Evaluation of hydrolysis as a function of pH
GLP:	Yes
Year:	2005
Method:	Hydrolytic stability determined at pH 4, 7, and 9 at 15°C and 25°C.
Results:	Half-life at pH 4 is 5159 and 179 days at 15 °C and 25°C respectively, at pH 7 is 87 and 26 days, and at pH 9 is 38 and 14 hours at 15 °C and 25 °C, respectively
Conclusions:	Fyrol 6 hydrolysis is both pH and temperature dependent
Reliability:	1
Reference:	7

### 3.4. Biodegradation:

Identity:	Fyrol 6; CAS# 2781-11-5; Batch 8106 J-5-2; purity not given
Method:	OECD 301D
Type:	Modified Sturm Test
GLP:	Yes

Year:	1990
% Degradation after 28 days:	15% (10 mg/L) and 19% (20 mg/L) at 28 days
Breakdown Products:	Not determined
Concentration Of Test Chemical:	10 mg/L, 20 mg/L
pH Of Test Media:	6.87-7.29
Conclusions:	Fyrol 6 is not readily biodegradable.
Reliability:	1
Reference:	8
Remarks:	Source of test organism was activated sludge obtained from a municipal sewage treatment plant

## 4. Ecotoxicity

### 4.1. Acute Toxicity to Fish:

Identity:	Fyrol 6; CAS# 2781-11-5; Batch 8106 J-5-2; purity not given
Method:	OECD 203
Type:	Static
GLP:	Yes
Year:	1990
Species/Strain:	Rainbow trout, <i>salmo gairdneri</i>
Supplier:	Hauxton Fishery Services, Cambridge, England
Analytical Monitoring:	None
Exposure Period:	96 hours
Nominal Concentrations:	1000, 1800, 3200, 5600 and 10000 mg/L
LC50:	>10000 mg/L
Conclusions:	The LC50 of Fyrol 6 is >10000 mg/L.
Reliability:	1
Reference:	9
Remarks:	There was 20% mortality at 3200 mg/L but none at higher concentrations. Ten fish were used in each test group. The water hardness was 216-242 mg/CaCO <sub>3</sub> /L. The pH was 7.08-8.32. The temperature was 14.1-15.0°C.

## 4.2. Acute Toxicity to Aquatic Invertebrates

Identity: Fyrol 6; CAS# 2781-11-5; Batch 04106G0101; Purity 84.5%  
Method: OECD 202 and EPA OPPTS 850.1010  
Type: Flow-through  
GLP: Yes  
Year: 2005  
Species/Strain: *Daphnia magna*  
Analytical Monitoring: Test substance concentration was measured in all chambers using a validated HPLC method  
Exposure Period: 48 hours  
Nominal Concentrations: 63, 125, 250, 500, and 1000 mg/L  
EC50: >936 mg/L  
Conclusions: The EC50 of Fyrol 6 is >936 mg/L.  
Reliability: 1  
Reference: 10  
Remarks: No treatment-related effects were observed at any concentration tested. The NOEC was 936 mg/l. The water hardness was 132 mg/CaCO<sub>3</sub>/L. The pH was 7.9-8.3. The temperature was 20.2°C throughout the test.

## 4.3 Acute Toxicity to Aquatic Plants

Identity: Fyrol 6; CAS# 2781-11-5; Lot T #150, Batch 04106G0101; Purity 84.5%  
Method: OECD 201 and EPA OPPTS 850.5400  
Type: 96 Hour Test under State Conditions  
GLP: Yes  
Year: 2006  
Species/Strain: *Pseudokirchneriella subcapitata*  
Analytical Monitoring: Test substance concentration was measured in all chambers using a validated HPLC method  
Exposure Period: 96 hours  
Nominal Concentrations: 7.5, 15, 30 60, and 120 mg/L  
EC50: >86 mg/L  
Conclusions: The EC50 of Fyrol 6 is >86 mg/L.  
Reliability: 1  
Reference: 11  
Remarks: No treatment-related effects were observed at any concentration tested. The NOEC was 86 mg/l. The temperature was maintained at 23 ± 2°C.

## 5. Mammalian Toxicity

### 5.1. Acute Toxicity:

#### 5.1.1. Oral

Identity: Fyrol 6; CAS# 2781-11-5; Lot# 2781115; purity not given  
Method: EPA Guidelines for pesticide registration; Fed. Reg. 43:163, 37336-37402 (1978); OECD (1981)  
Type: Acute Oral LD50  
GLP: Yes  
Year: 1983  
Species/Strain: Rat/Sprague-Dawley  
Sex: M/F  
No. Of Animals Per Sex Per Dose: 10  
Vehicle: Corn oil  
Route Of Administration: Oral gavage  
Time Of Observation Period: 14 Days  
Doses Administered: 5000 mg/kg  
LD50: >5000 mg/kg  
Conclusions: The oral LD50 of Fyrol 6 in rats is greater than 5000 mg/kg.  
Reliability: 1  
Reference: 12  
Remarks: Clinical signs of toxicity were mild depression, piloerection, alopecia and red facial stains. All animals appeared normal by day 2.

#### 5.1.2. Dermal

Identity: Fyrol 6; CAS# 2781-11-5; Lot# 2781115; purity not given  
Method: EPA Guidelines for pesticide registration; Fed. Reg. 43:163, 37336-37402 (1978); OECD (1981)  
Type: Acute Dermal  
GLP: Yes  
Year: 1983  
Species/Strain: Rabbit/Stauffland albino  
Sex: M/F

No. Of Animals Per 5  
 Sex Per Dose:  
 Vehicle: None  
 Route Of Administration: Dermal  
 Time Of Observation Period: 14 Days  
 Doses Administered: 2000 mg/kg for 24 hours  
 LD50: >2000 mg/kg  
 Conclusions: The dermal LD50 of Fyrol 6 in rabbits is greater than 2000 mg/kg.  
 Reliability: 1  
 Reference: 13  
 Remarks: There was no mortality. Clinical signs of toxicity were mild depression. All animals appeared normal by day 2. Local dermal effects included mild erythema and edema. There were no adverse effects at necropsy.

### 5.1.3. Skin Irritation

Identity: Fyrol 6; CAS# 2781-11-5; Lot# 2781115; purity not given  
 Method: DOT Fed. Reg. Title 49, Part 173 Appendix II 10/1/77  
 Type: Skin irritation  
 GLP: Yes  
 Year: 1983  
 Species/Strain: Rabbit/Stauffland albino  
 Sex: M/F  
 No. Of Animals: 6  
 Vehicle: None  
 Route Of Administration: Dermal  
 Time Of Exposure: 4 hours  
 Time Of Observation Period: 4 and 48 hours  
 Volume Administered: 0.5mL  
 Results: There was no erythema or edema at any observation period. Draize scoring used.  
 Conclusions: Fyrol 6 was not irritating to rabbits following dermal exposure for 4 hours.  
 Reliability: 1

Reference: 14

#### 5.1.4. Eye Irritation

Identity: Fyrol 6; CAS# 2781-11-5; Lot# 2781115; purity not given

Method: EPA Guidelines for pesticide registration; Fed. Reg. 43:163, 37336-37402 (1978); OECD (1981)

Type: Eye irritation

GLP: Yes

Year: 1983

Species/Strain: Rabbit/Stauffland albino

Sex: M/F

No. Of Animals: 9

Vehicle: None

Route Of Administration: Ocular

Time Of Exposure: Eyes of 3 animals washed after 20-30 seconds of exposure. Eyes of the other 6 animals were not washed.

Time Of Observation: 24, 48, 72 hours and 4, 7 days

Period:

Concentration Of Test Material: 0.1mL

Results: There was mild conjunctival irritation in 6 rabbits with unwashed eyes and no effects in the 3 rabbits with washed eyes. The irritation cleared by the 72 hour observation period. Draize scoring used.

Conclusions: Fyrol 6 was mildly irritating to rabbits.

Reliability: 1

Reference: 15

#### 5.2. Repeated Dose Toxicity:

Identity: Fyrol 6; CAS# 2781-11-5; Lot# 1106 L-1; purity – 90.7%

Method: Repeat Dose - Oral

Type: 13-Week Oral Toxicity

GLP: Yes

Year: 1983

Species/Strain: Rat/Sprague-Dawley

Sex: M/F

No. Of Animals Per Sex Per Dose: 22

Vehicle: Corn oil

Route of Administration:	Oral gavage
Time of Observation Period:	13 weeks
Doses Administered:	20, 100, 500 mg/kg/day
Frequency of Treatment:	Once daily for 13 weeks, 7 days per week
NOAEL:	500 mg/kg/day
LOAEL:	>500 mg/kg/day
Toxic Response By Dose Level:	Control: Mortality - three females (dosing accident) and three males (dosing accident); Macroscopic exam - enlarged liver in eight animals. 500 mg/kg/day: Mortality - one male (dosing accident) and six females (dosing accident); Clinical signs - alopecia, darker coloration of eyes, chromorhinorrhea; Clinical chemistry - increase in white blood cells; lower hemoglobin and hematocrit; Macroscopic exam - discoloration of lungs, thymus, liver and kidney and enlarged liver; Organ weights - significant increase in mean absolute and relative liver weight and an increase in mean absolute and relative kidney weight; Microscopic exam - very slight hepatocellular hypertrophy, cytoplasmic eosinophilia of centrilobular hepatocytes. 100 mg/kg/day - Mortality - five males (dosing accident) and two females (dosing accident); Clinical signs - alopecia; Clinical chemistry - decrease in red blood cells; Macroscopic exam - discoloration of lungs, liver and kidney and enlarged liver; Organ weights - increase in mean relative liver and absolute and relative kidney weight; Microscopic exam - very slight hepatocellular hypertrophy, cytoplasmic eosinophilia of centrilobular hepatocytes. 20 mg/kg/day - Mortality - One male (dosing accident) and three females (dosing accident); Clinical signs - alopecia; Clinical chemistry - decrease in red blood cells; Macroscopic exam - discoloration of lungs and kidney and enlarged liver; Organ weights - no changes; Microscopic exam - no changes. There were no signs of functional changes in the kidney and liver of animals in any dose groups.
Conclusions:	Fyrol 6 administered daily by oral gavage to rats for 13 weeks resulted in minor histopathological changes in the liver at doses of 100 and 500 mg/kg/day. These results were considered an adaptive rather than a toxic response to Fyrol 6. The NOAEL was 500 mg/kg/day.
Reliability:	1
Reference:	16

### 5.3. Genetic Toxicity:

#### 5.3.1. *In Vitro* Gene Mutations

Identity: Fyrol 6; CAS# 2781-11-5; Lot # 49; purity not given  
Method: Ames test  
Type: Reverse mutation assay  
GLP: Yes  
Year: 1978  
Cell Type: Salmonella typhimurium TA1535, TA1537, TA 1538, TA98, TA100; S. cerevisiae D4  
Metabolic Activation: Rat and mouse S9 induced by Aroclor 1254 or phenobarbital  
Concentrations Tested: With/Without S9: 0.01-10 ul/plate  
Vehicle: Dimethyl sulfoxide  
Cytotoxic Concentration: No toxicity at any concentration.  
Genotoxic Effects With Metabolic Activation: None  
Genotoxic Effects Without Metabolic Activation: None  
Conclusions: Fyrol 6 was not mutagenic in Salmonella typhimurium strains TA1535, TA1537, TA1538, TA98, TA100 or S. cerevisiae strain D4 in the presence or absence of metabolic activation.  
Reliability: 1  
Reference: 17

Identity: Fyrol 6; CAS# 2781-11-5; Lot # 49; purity not given  
Method: Mouse lymphoma assay  
Type: Forward mutation assay  
GLP: Yes  
Year: 1978  
Cell Type: Mouse lymphoma cell line L5178Y  
Metabolic Activation: Rat S9 induced by Aroclor 1254  
Concentrations Tested: With S9: 0.626-2.5 uL/mL  
Without S9: 1.25-5 ul/mL  
Vehicle: Sterile water

Cytotoxic Concentration:	Cytotoxic at 2.5 and 5 ul/mL
Genotoxic Effects With Metabolic Activation:	Weakly mutagenic
Genotoxic Effects Without Metabolic Activation:	Weakly mutagenic
Conclusions:	Fyrol 6 was weakly mutagenic in the presence and absence of metabolic activation.
Reliability:	1
Reference:	18

Identity:	Fyrol 6; CAS# 2781-11-5; Lot # 1106C-1-3; purity not given
Method:	Mouse lymphoma assay
Type:	Forward mutation assay
GLP:	Yes
Year:	1981
Cell Type:	Mouse lymphoma cell line L5178Y
Metabolic Activation	Rat S9 induced by Aroclor 1254
Concentrations Tested:	With S9: 0.25-1.0 uL/mL Without S9: 0.0313-0.5 ul/mL
Vehicle:	Sterile water
Cytotoxic Concentration:	Cytotoxic at 0.5 ul/mL
Genotoxic Effects With Metabolic Activation:	Weakly mutagenic
Genotoxic Effects Without Metabolic Activation:	Weakly mutagenic
Conclusions:	Fyrol 6 was weakly mutagenic in the presence and absence of metabolic activation.
Reliability:	1
Reference:	19

### 5.3.2 *In Vitro* Chromosome Aberrations

Identity:	Fyrol 6; CAS# 2781-11-5; Lot # 1106C-1-3; purity not given
Method:	Mouse lymphoma assay
Type:	Chromosome aberration

GLP:	Yes
Year:	1982
Cell Type:	Mouse lymphoma cell line L5178Y
Metabolic Activation	Rat S9 induced by Aroclor 1254
Concentrations Tested:	With S9: 0.25-2.0 uL/mL Without S9: 0.0313-0.5 ul/mL
Vehicle:	Sterile water
Cytotoxic Concentration:	None
Genotoxic Effects With Metabolic Activation:	Clastogenic. Both structural and numerical chromosome aberrations were seen in the two highest dose groups.
Genotoxic Effects Without Metabolic Activation:	Clastogenic. Both structural and numerical chromosomal aberrations were seen in the two highest dose groups.
Conclusions:	Fyrol 6 was clastogenic in the presence and absence of metabolic activation.
Reliability:	1
Reference:	20
Remarks:	A statistically significant increase in structural and numerical aberrations was reported.

### 5.3.3 *In Vitro* Transformation

Identity:	Fyrol 6; CAS# 2781-11-5; Lot # 49; purity not given
Method:	BALB/3T3 Cell assay
Type:	In vitro transformation assay
GLP:	Yes
Year:	1978
Cell Type:	BALB/3T3 cells
Metabolic Activation	Not applicable
Concentrations Tested:	0.02-0.312 uL/mL
Vehicle:	Medium
Cytotoxic Concentration:	None
Genotoxic Effects With Metabolic Activation:	None
Genotoxic Effects Without Metabolic Activation:	None

Conclusions: Fyrol 6 was not active in this assay.  
Reliability: 1  
Reference: 21  
Remarks: The cells were examined after a 72 hour exposure period and 3-4 week growth period

## 5.4 Reproductive/Developmental Toxicity

Identity: Fyrol 6; CAS# 2781-11-5; Lot# 04106C0103; Purity 85%  
Type/Guideline: Reproductive/Developmental Screen OECD 421  
GLP: Yes  
Year: 2006  
Species/Strain: Rat/Sprague-Dawley  
Sex: M/F  
No. Of Animals Per Sex Per Dose: 12 per sex per dose group  
Vehicle: Water  
Route of Administration: Oral gavage  
Time of Observation: Various times throughout study, evaluating different endpoints  
Period: Various times throughout study, evaluating different endpoints  
Doses Administered: 50, 250, or 750 mg/kg/day  
Frequency of Treatment: Once daily  
NOAEL: 750 mg/kg/day  
LOAEL: >750 mg/kg/day  
Results: Fyrol 6 was administered daily for two weeks prior to mating, during the mating period, through gestation and lactation, and until sacrifice. Parental body weights, food consumption, body weight gain, reproductive performance, organ weights, and histopathology were evaluated during the study. Offspring survival and body weights were also measured. There were no treatment-related clinical signs or mortality. Parental body weights and food consumption were unaffected by treatment. There were no significant differences in mean corpora lutea, implantation sites, litter size, total pups born, and pup survival. Offspring body weights were similar across dose groups and were unaffected by treatment. Parental reproductive organ weights (ovaries, testes, or epididymides) were unaffected. Male liver weights and liver-to-body weight ratios were increased in a dose-

related manner; however, statistical significance was not achieved. There was no evidence of histological changes in the reproductive organs. Based on these findings, the NOAEL for reproductive toxicity of Fyrol 6 is equal to or greater than 750 mg/kg/day.

Reliability 1  
Reference 22

## 5.5 Neurotoxicity

Identity: Fyrol 6; CAS# 2781-11-5; Lot# 0106E-2-2; purity – 97.4%  
Method: Fed. Reg. 43 (163):37362-37363, 1978  
Type: Acute Delayed Neurotoxicity  
GLP: Yes  
Year: 1982  
Species/Strain: Hen/White Leghorn  
Sex: F  
No. Of Animals Per Sex Per Dose: 10  
Vehicle: Corn oil  
Route of Administration: Oral gavage  
Time of Observation: 43 Days  
Period:  
Doses Administered: 1 or 10 g/kg  
Frequency of Treatment: Two doses, three weeks apart  
NOAEL (NOEL): 10 g/kg x 2  
LOAEL (LOEL): None  
Toxic Response By Dose Level: None  
Conclusions: Fyrol 6 administered to hens did not cause delayed neurotoxicity at doses up to 10 g/kg administered 3 weeks apart.  
Reliability: 1  
Reference: 23  
Remarks: Tri-ortho-cresyl phosphate was used as the positive control. Clinical and histopathology evaluations were conducted.

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