BPD/BPA Coalition

BPD/BPA Coalition

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BPD (Benzene Phosphorous Dichloride) Robust Summaries

Submitted to the U.S. Environmental Protection Agency

by the

BPD/BPA Coalition

November, 2003

20031119075800.

BPD/BPA Coalition

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1. Substance Information

CAS Number:	**644-97-3**
Chemical Name:	Phosphonous dichloride, phenyl-
Structural Formula:	$C_6H_5Cl_2P$
Other Names:	**BPD,** Benzene phosphorus dichloride
Exposure Limits:	Not established

2. Physical – Chemical Properties

2.1. Melting Point:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available
GLP:	No data available
Year:	No data available
Value:	-51 °C
Decomposition:	No data available
Conclusions:	A handbook value for the melting point of BPD is -51 °C
Reliability:	1
Reference:	CRC Handbook of Chemistry and Physics, 75th edition (1944) CRC Press, Boca Raton.
Remarks:	Handbook value
Additional References for Melting Point Studies:	None

2.2. Boiling Point:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available
GLP:	No data available
Year:	No data available
Value:	225 °C
Pressure:	No data available
Pressure Unit:	No data available
Decomposition:	Not described
Conclusions:	The boiling point of BPD is 225 °C
Reliability:	4

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Reference:	Avecia, Inc. (1998) BPD Refined (Benzene Phosphorus Dichloride) MSDS, revision D, issued 9/24/98
Remarks:	None
Additional References for Boiling Point Studies:	None

2.3. Density:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available
GLP:	No data available
Year:	No data available
Value:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Density Studies:	None

2.4. Vapor Pressure:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available
GLP:	No data available
Year:	No data available
Value:	10
Temperature° C:	98
Pressure Unit:	mmHg
Decomposition:	No data available
Conclusions:	The vapor pressure of BPD is 10 at 98 °C
Reliability:	4
Reference:	Avecia, Inc. (1998) BPD Refined (Benzene Phosphorus Dichloride) MSDS, revision D, issued 9/24/98
Remarks:	None
Additional Reference for Vapor Pressure Studies:	None

2.5. Partition Coefficient (log Kow):

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	Not applicable
GLP:	Not applicable

Year:	Not applicable
Log Kow:	Decomposes
Temperature°C:	Not applicable
Conclusions:	Not applicable
Reliability:	Not applicable
Reference:	Not applicable
Remarks:	Rapidly hydrolyzes
Additional References for Partition Coefficient Studies:	None

2.6. Water Solubility:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	Not applicable
GLP:	Not applicable
Year:	Not applicable
Value at temperature°C:	Not applicable
Description of solubility:	Decomposes
PH value and concentration at temperature °C:	Not applicable
Pka value at 25°C:	Not applicable
Conclusions:	Rapidly hydrolyzes
Reliability:	Not applicable
Reference:	Not applicable
Remarks:	Decomposes
Additional References for Water Solubility Studies:	None

2.7. Flash Point:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available
GLP:	No data available
Year:	No data available
Results:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None

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Additional References for Flash Point Studies:	None

2.8. Flammability:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available
GLP:	No data available
Year:	No data available
Results:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Flammability Studies:	None

3. Environmental Fate

3.1. Photodegradation:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	EPIWIN Model calculation: (AopWin v1.90)
GLP:	Not applicable
Type:	Model calculation
Year:	2003
Light Source:	Not applicable
Light Spectrum (nm):	Not applicable
Half-life:	65.8 hours (5.5 days for 12 hour days)
Breakdown Products:	No data available
Conclusions:	The half-life in the atmosphere for BPA is estimated to be 65.8 hours (5.5 days for 12 hour days)
Reliability	1
Reference:	AOP Version 1.90
Remarks:	None
Additional References for Photodegradation Studies:	None

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3.2. Stability in Water:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	OECD 111
GLP:	Yes
Type:	Laboratory study
Year:	2003
Half-life at a specific pH:	< 1 minute at pH 1.2, 4, 7, and 9 at 25 °C
Breakdown Products:	BPA, phenylphosphonic acid, phenylphosphine, Cl^-
Conclusions:	Rapidly hydrolyzed
Reliability:	1
Reference:	Wildlife International, Ltd. (2003) Hydrolytic stability of benzene phosphonous dichloride. Project number 534C-123.
Remarks:	The industrial process gives a high >95% yield of BPA, but under the OECD 111 conditions, the yield of BPA and PPOA is approximately the same
Additional References for Stability in Water Studies:	None

3.3. Transport (Fugacity):

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	EPIWIN Model calculation (Level III Fugacity Model)
GLP:	No
Type:	Model calculation
Year:	2003
Media:	Air, Water, Soil, Sediment

Distributions:

Compartment	Released 100% to air	Release 100% to water	Release 100% to soil
Air	79.8	0.889	0.0736
Water	12.7	98	0.792
Soil	7.3	0.0813	99.1
Sediment	0.139	1.07	0.00865

Adsorption Coefficient:	No data available
Desorption:	No data available
Volatility:	No data available
Conclusions:	Partitions primarily to soil and water. In the presence of water, BPD will rapidly hydrolyze.
Reliability:	1
Reference:	EPIWIN (version 3.1) STP Fugacity model

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Remarks:	When released equally to air, water, and soil, BPD is estimated to be distributed 7.15 percent to air, 36.7 percent to water, 55.8 percent to soil, and 0.401 percent to sediment
Additional References for Transport (Fugacity) Studies:	None

3.4. Biodegradation:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	EPIWIN 3.10 (BIOWIN v4.00)
Type:	Model calculation
GLP:	No
Year:	2003
Degradation% after time:	No data available
Breakdown Products:	Hydrolysis products are BPA, PPOA, and phenylphosphine
Concentration Of Test Chemical:	No applicable
Analytical Method:	Not applicable
Conclusions:	Ultimate Biodegradation Timeframe: weeks Primary Biodegradation Timeframe: days-weeks
Reliability:	1
Reference:	BIOWIN v 4.00
Remarks:	BIOWIN fragment descriptor is for an unsubstituted phenyl group
Additional References for Biodegradation Studies:	None

3.5. Bioconcentration:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	EPIWIN 3.10 (Bcfwin v2.14)
Type:	Model calculation
GLP:	No
Year:	2003
Results:	Log BCF = 1.62 (BCF = 41.72)
Conclusions:	Not expected to bioaccumulate
Reliability:	1
Reference:	Bcfwin Version 2.14
Remarks:	None

Additional References for Bioconcentration Studies:	None

4. Ecotoxicity

4.1. Acute Toxicity to Fish:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	EPIWIN 3.10 (ECOSAR Version 0.99)
Type:	Model calculation
GLP:	No
Year:	2003
Species/Strain/:	Not applicable
Supplier:	Not applicable
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Nominal/Measured Concentrations:	Not applicable
LC50:	14.908 mg/L at 96 hours
Conclusions:	Predicted to be slightly toxic to fish
Reliability:	1
Reference:	ECOSAR version 0.99
Remarks:	None
Additional References for Acute Toxicity to Fish Studies:	None

4.2. Acute Toxicity to Invertebrates:.

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	EPIWIN 3.10 (ECOSAR version 0.99)
Type:	Model calculation
GLP:	No
Year:	2003
Species/Strain/:	Daphnid
Supplier:	Not applicable
Analytical Monitoring:	Not applicable
Exposure Period:	48 hours
Nominal/Measured Concentrations:	Not applicable
LC50:	17.129 mg/L at 96 hours

Conclusions:	Predicted to be slightly toxic to aquatic organisms
Reliability:	1
Reference:	ECOSAR version 0.99
Remarks:	None
Additional References for Acute Toxicity to Invertebrates Studies:	None

4.3. Acute Toxicity to Aquatic Plants:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	EPIWIN 3.10 (ECOSAR version 0.99)
Type:	Model calculation
GLP:	No
Year:	2003
Species/Strain/ Supplier:	Green algae
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Nominal/Measured Concentrations:	Not applicable
EC50:	11.349 mg/L in green algae at 96 hours
Conclusions:	Predicted to be slightly toxic to green algae
Reliability:	1
Reference:	ECOSAR version 0.99
Remarks:	None
Additional References for Acute Toxicity to Aquatic Plants Studies:	None

5. Mammalian Toxicity

5.1. Acute Toxicity:

5.1.1. Oral

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	OECD 420 Fixed dose
Type:	Guideline
GLP:	Yes
Year:	1997
Species/Strain:	Alpk: Ap_fSD (Wistar-derived)

Sex:	Male and female
No. Of Animals Per Sex Per Dose:	5
Vehicle:	Corn oil
Route Of Administration:	Oral gavage
Time Of Observation Period:	14 days
Doses Administered:	1
LD50:	> 500 mg/kg
Conclusions:	No mortality in the dosed animals at 500 mg/kg. The one rat tested at 2000 mg/kg in the rangefinding test died
Reliability:	1
Reference:	Astra Zeneca Central Toxicology Laboratory (1977) Report number CTL/P/5737. Benzene phosphorous dichloride – refined: Fixed dose acute oral toxicity to the rat
Remarks:	According to the study report, there were no signs of evident toxicity and all animals showed an overall body weight gain during the study. Two male animals had mottled lungs and froth in the trachea at necropsy which may be treatment related. The necropsy data, however, supports the conclusion that the administered BPD was hydrolyzed in vivo, presumably to the relatively strong acids BPA and BPD and that these compounds caused their characteristic effect – gastrointestinal bleeding. The single animal dosed with 2000 mg/kg died on the first day and the necropsy comment was, "stomach and intestine contents dark (black). In addition, all 5 males dosed at 500 mg/kg where noted to have "slight" scores for "activity decreased" on the day of dosing. This is consistent with the interpretation that the hydrolysis products produced gastrointestinal irritation and possible distress. The absence of gastrointestinal findings at necropsy in the 500 mg/kg animals may be attributed to healing.
Additional References for Acute Oral Toxicity Studies:	None

5.1.2. Dermal

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available

Type:	No data available
GLP:	No data available
Year:	No data available
Species/Strain:	No data available
Sex:	No data available
No. Of Animals Per Sex Per Dose:	No data available
Vehicle:	No data available
Route Of Administration:	No data available
Time Of Observation Period:	No data available
Doses Administered:	No data available
LD50:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Acute Dermal Toxicity Studies:	None

5.1.3. Irritation

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Species/Strain:	No data available
Sex:	No data available
No. Of Animals Per Sex Per Dose:	No data available
Vehicle:	No data available
Route Of Administration:	No data available
Time Of Observation Period:	No data available
Concentration Of Test Material:	No data available
Results:	No data available
Conclusions:	No data available

Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Acute Dermal Irritation Studies:	None

5.1.4. Sensitization

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Species/Strain:	No data available
Sex:	No data available
No. Of Animals Per Sex Per Dose:	No data available
Vehicle:	No data available
Route Of Administration:	No data available
Time Of Observation Period:	No data available
Concentration Of Test Material:	No data available
Results:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Acute Dermal Sensitization Studies:	None

5.1.5. Eye Irritation

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Species/Strain:	No data available
No data available	No data available

Sex:	
No. Of Animals Per Sex Per Dose:	No data available
Vehicle:	No data available
Route Of Administration:	No data available
Time Of Observation Period:	No data available
Concentration Of Test Material:	No data available
Results:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Acute Eye Irritation Studies:	None

5.2. Repeated Dose Toxicity:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Species/Strain:	No data available
Sex:	No data available
No. Of Animals Per Sex Per Dose:	No data available
Vehicle:	No data available
Route of Administration:	No data available
Time of Observation Period:	No data available
Doses Administered:	No data available
Frequency of Treatment:	No data available
NOAEL (NOEL):	No data available
LOAEL (LOEL):	No data available
Toxic Response By Dose Level:	No data available

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Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Repeated Dose Toxicity Studies:	None

5.3. Reproductive Toxicity:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Species/Strain:	No data available
Sex:	No data available
No. Of Animals Per Sex Per Dose:	No data available
Vehicle:	No data available
Route Of Administration:	No data available
Time Of Observation Period:	No data available
Doses Administered:	No data available
Frequency Of Treatment:	No data available
Premating Exposure For Males:	No data available
Premating Exposure For Females:	No data available
P NOAEL (NOEL):	No data available
P LOAEL (LOEL):	No data available
F1 NOAEL (NOEL):	No data available
F1 LOAEL (LOEL);	No data available
F2 NOAEL (NOEL):	No data available
F2 LOAEL	No data available

(LOEL):	
P/F1/F2 Toxic Response By Dose Level:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Reproductive Toxicity Studies:	None

5.4. Genetic Toxicity:

5.4.1. *In Vitro* Gene Mutations

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	OECD 471, OECD 472
Type:	Guideline
GLP:	Yes
Year:	1997
Cell Type:	TA1535, TA1537, TA98, TA100, WP2P, WP2P*uvrA*
Metabolic Activation:	S9 was prepared from male Sprague-Dawley rats dosed once dialy by oral gavage with a combined Phenobarbital (80 mg/gk) and β-napthoflavone (100 mg/kg) in corn oil
Concentrations Tested:	50, 100, 200, 500, 1000, 2500 µg/ plate
Vehicle:	DMSO
Cytotoxic Concentration:	2500 µg/ plate (background lawn sparse/absent)
Genotoxic Effects With Metabolic Activation:	Increased revertents with WP2P and TA98
Genotoxic Effects Without Metabolic Activation:	Increased revertents with WP2P
Conclusions:	Mutagenic
Reliability:	1
Reference:	Astra Zeneca Central Toxicology Laboratory (1977) Report number CTL/P/5678. Benzene phosphorous dichloride: Bacterial mutation assay in *S. typhimurium* and *E. coli*
Remarks:	None

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Additional References for In Vitro Gene Mutation Studies:	None

5.4.2. *In Vitro* Chromosome Aberrations

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Cell Type:	No data available
Metabolic Activation	No data available
Concentrations Tested:	No data available
Vehicle:	No data available
Cytotoxic Concentration:	No data available
Genotoxic Effects With Metabolic Activation:	No data available
Genotoxic Effects Without Metabolic Activation:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for *In Vitro* Chromosome Aberration Studies:	None

5.4.3. *In Vivo* Chromosome Aberrations

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Species/Strain:	No data available
Sex:	No data available
Route Of Administration:	No data available
Vehicle:	No data available

Doses Administered:	No data available
Genotoxic Effects:	No data available
NOAEL (NOEL):	No data available
LOAEL (LOEL):	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for *In Vivo* Chromosome Aberration Studies:	None

5.5. Developmental Toxicity:

Identity:	BPD (phosphonous dichloride, phenyl-) CAS#: 644-97-3
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Species/Strain:	No data available
Sex:	No data available
No. Of Animals Per Sex Per Dose:	No data available
Vehicle:	No data available
Route Of Administration:	No data available
Time Of Observation Period:	No data available
Doses Administered:	No data available
Frequency Of Treatment:	No data available
Maternal NOAEL (NOEL):	No data available
Maternal LOAEL (LOEL):	No data available
Fetal NOAEL (NOEL):	No data available
Fetal LOAEL (LOEL):	No data available
Maternal Toxic Response By Dose Level:	No data available

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Fetal Toxic Response By Dose Level:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Developmental Toxicity Studies:	None

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BPA (Benzene Phosphinic Acid) Robust Summaries

Submitted to the U.S. Environmental Protection Agency

by the

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November, 2003

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1. Substance Information

CAS Number:	1779-48-2
Chemical Name:	Phosphinic acid, phenyl
Structural Formula:	$C_6H_7O_2P$
Other Names:	BPA, benzene phosphinic acid
Exposure Limits:	Not established

2. Physical – Chemical Properties

2.1. Melting Point:

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	No data available
GLP:	No data available
Year:	No data available
Value:	83 °C
Decomposition:	No data available
Conclusions:	The melting point of BPA is 83 °C
Reliability:	4
Reference:	Akzo Nobel Functional Chemicals LLC (2000) BPA MSDS revision 3, revised 7/12/2000
Remarks:	None
Additional References for Melting Point Studies:	None

2.2. Boiling Point:

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	No data available
GLP:	No data available
Year:	No data available
Value:	180 °C
Pressure:	760
Pressure Unit:	mmHg
Decomposition:	No data available
Conclusions:	The boiling point of BPA is 180 °C
Reliability:	4

Reference:	Acros Organics MSDS Phenylphosphonic acid. Revision: 2/18/2002
Remarks:	None
Additional References for Boiling Point Studies:	None

2.3. Density:

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	No data available
GLP:	No data available
Year:	No data available
Value:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Density Studies:	None

2.4. Vapor Pressure:

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	Model calculation
GLP:	No
Year:	2003
Value:	0.00014
Temperature° C:	25 °C
Pressure Unit:	mmHg
Decomposition:	No data available
Conclusions:	The vapor pressure of BPA is 0.00014 mmHg
Reliability:	1
Reference:	MBPWIN Version 1.40
Remarks:	None
Additional Reference for Vapor Pressure Studies:	None

2.5. Partition Coefficient (log Kow):

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	Model calculation
GLP:	No
Year:	2003

Log Kow:	0.04
Temperature°C:	No data available
Conclusions:	The log Kow of BPA is estimated to be 0.04
Reliability:	1
Reference:	WSKOW version 1.40
Remarks:	None
Additional References for Partition Coefficient Studies:	None

2.6. Water Solubility:

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	No data available
GLP:	No
Year:	2003
Value at temperature°C:	77,000 mg/L @25° C
Description of solubility:	No data available
PH value and concentration at temperature °C:	pH = 1 at 25 °C for a saturated solution pH = 2 for a 1% solution
pka value at 25°C:	1.35, 1.92
Conclusions:	The soluability of BPA is 77,000 mg/L @25° C
Reliability:	4
Reference:	Akzo Nobel Functional Chemicals LLC (2000) BPA MSDS revision 3, revised 7/12/2000
Remarks:	pH of saturated solution is 1. Akzo Nobel Chemicals Project 6017000, 6/19/03. pH of a 1% solution is 2. Acros Organics MSDS Phenylphosphonic acid. Revision: 2/18/2002
Additional References for Water Solubility Studies:	PKa reference: Morelli, J.J. (2003) Technical Information Report 31118. Akzo Nobel Chemicals, Inc. Dobbs Ferry, NY.

2.7. Flash Point:

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	No data available
GLP:	No data available
Year:	No data available
Results:	No data available
Conclusions:	No data available
Reliability:	No data available

Reference:	No data available
Remarks:	None
Additional References for Flash Point Studies:	None

2.8. *Flammability:*

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	No data available
GLP:	No data available
Year:	No data available
Results:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Flammability Studies:	None

3. Environmental Fate

3.1. *Photodegradation:*

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	EPIWIN Model calculation: (AopWin v1.90)
GLP:	No
Type:	Model calculation
Year:	2003
Light Source:	Not applicable
Light Spectrum (nm):	Not applicable
Half-life:	61.4 hours (5.1 days for 12 hour days)
Breakdown Products:	No data available
Conclusions:	The half-life of BPA in the atmosphere is 61.4 hours (5.1 days for 12 hour days)
Reliability	1
Reference:	AOP Version 1.90
Remarks:	None
Additional References for Photodegradation Studies:	None

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3.2. Stability in Water:

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	No data available
GLP:	No data available
Type:	No data available
Year:	No data available
Half-life at a specific pH:	No data available
Breakdown Products:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Stability in Water Studies:	None

3.3. Transport (Fugacity):

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	EPIWIN Model calculation STP Fugacity model
GLP:	No
Type:	Model calculation
Year:	2003
Media:	Air, Water, Soil, Sediment

Distributions:

Compartment	Released 100% to air	Release 100% to water	Release 100% to soil
Air	0.118	7.11e-007	0.000175
Water	27.4	99.8	21.6
Soil	72.4	0.000438	78.4
Sediment	0.0461	0.168	0.0363

Adsorption Coefficient:	No data available
Desorption:	No data available
Volatility:	No data available
Conclusions:	Partitions primarily to soil and water
Reliability:	1
Reference:	EPIWIN (version 3.1) STP Fugacity model
Remarks:	When released equally to air, water, and soil, BPA is estimated to be distributed 0.0422 percent to air, 44.9 percent to water, 55 percent to soil, and 0.0755 percent to sediment

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Additional References for Transport (Fugacity) Studies:	None

3.4. Biodegradation:

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	EPIWIN 3.10 (BIOWIN v4.00)
Type:	Model calculation
GLP:	No
Year:	2003
Degradation% after time:	No data available
Breakdown Products:	No data available
Concentration Of Test Chemical:	No data available
Analytical Method:	No applicable
Conclusions:	Ultimate Biodegradation Timeframe: weeks Primary Biodegradation Timeframe: days-weeks
Reliability:	1
Reference:	BIOWIN Version 4.00
Remarks:	None
Additional References for Biodegradation Studies:	None

3.5. Bioconcentration:

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	EPIWIN 3.10 (Bcfwin v2.14)
Type:	Model calculation
GLP:	No
Year:	2003
Results:	Log BCF = 0.5 (BCF = 3.162)
Conclusions:	Not expected to bioaccumulate
Reliability:	1
Reference:	Bcfwin Version 2.14
Remarks:	None
Additional References for Bioconcentration Studies:	None

4. Ecotoxicity

4.1. Acute Toxicity to Fish:

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	EPIWIN 3.10 (ECOSAR Version 0.99)
Type:	Model calculation
GLP:	No
Year:	2003
Species/Strain/:	Not applicable
Supplier:	Not applicable
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Nominal/Measured Concentrations:	Not applicable
LC50:	9721.6 mg/L
Conclusions:	Predicted to be practically nontoxic to fish
Reliability:	1
Reference:	ECOSAR Version 0.99
Remarks:	None
Additional References for Acute Toxicity to Fish Studies:	None

4.2. Acute Toxicity to Invertebrates:.

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	EPIWIN 3.10 (ECOSAR version 0.99)
Type:	Model calculation
GLP:	No
Year:	2003
Species/Strain/:	Daphnid
Supplier:	Not applicable
Analytical Monitoring:	No applicable
Exposure Period:	48 hours
Nominal/Measured Concentrations:	Not applicable
LC50:	6857.7 mg/L
Conclusions:	Predicted to be practically nontoxic to invertebrates
Reliability:	1
Reference:	ECOSAR version 0.99
Remarks:	None

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Additional References for Acute Toxicity to Invertebrates Studies:	None

4.3. Acute Toxicity to Aquatic Plants:

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	EPIWIN 3.10 (ECOSAR version 0.99)
Type:	Model calculation
GLP:	No
Year:	2003
Species/Strain/ Supplier:	Green algae
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Nominal/Measured Concentrations:	Not applicable
EC50:	3829.8 mg/L
Conclusions:	Predicted to be practically non toxic to green algae
Reliability:	1
Reference:	ECOSAR version 0.99
Remarks:	None
Additional References for Acute Toxicity to Aquatic Plants Studies:	None

5. Mammalian Toxicity

5.1. Acute Toxicity:

5.1.1. Oral

Identity:	BPA (PHOSPHINIC ACID, PHENYL-) CAS# 1779-48-2
Method:	Fixed dose
Type:	Acute oral gavage
GLP:	No
Year:	1969
Species/Strain:	Rat, not specified
Sex:	Male and female
No. Of Animals Per Sex Per Dose:	5
Vehicle:	Water (assumed), 1% tragacanth, 0.5% Tween 20

Route Of Administration:	Oral (gavage assumed)
Time Of Observation Period:	14 days
Doses Administered:	Females: 464, 1000, 2150 mg/kg as 10% concentration of BPA Males: 1000, 2150, (as 10% concentration of BPA) 4640 mg/kg as 25% concentration of BPA
LD50:	1710 mg/kg for male rats and 1470 mg/kg for female rats
Conclusions:	Females: No apparent toxicity at 464 mg/kg. At necropsy, the 464 mg/kg animals appeared grossly normal. At 1000 mg/kg 5 of 5 animals survided. There was acute depression, dark soft stool, and periods of erratic excitation. At 2150 mg/kg, 5 0f 5 animals died between 6 and 10 hours after dosing. At necropsy, gastrointestinal hemorrhage was noted. Males: The 1000 mg/kg level had no mortality but produced depression subsiding after 48-96 hours. Higher levels produced dark soft stool and acute depression with periods of excitation. At necropsy these animals had areas of necrotic tissue in the gastrointestinal tract. At 2150 mg/kg, 4 of 5 males died between 10 and 14 hours after dosing. At necropsy, the survivor had areas of necrotic tissue in the gastrointestinal tract. At 4640 mg/kg, 5 of 5 males died between 3 and 5 hours after dosing. Necropsy findings describe extensive areas of gastrointestinal hemorrhage.
Reliability:	3
Reference:	Stuaffer Chemical Company (1968) Toxicology Lab Report T-1233 Benzene Phosphinic Acid
Remarks:	The clinical signs described and the necropsy results are consistent with the interpretation that these animals died as a result of the strong acid properties of BPA causing gastrointestinal bleeding and death as a consequence. The clinical signs, in particular, are consistent with the interpretation that these animals probably experienced significant distress.
Additional References for Acute Oral Toxicity Studies:	Haskell Data MR-1703-013, HL-0009-54 cited in Microfiche OTS 05555311 (1992). Eastman Kodak Co, TSCA 8e submission.

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5.1.2. Dermal

Identity:	BPA (PHOSPHINIC ACID, PHENYL-) CAS# 1779-48-2
Method:	Occluded patch
Type:	Acute 24 hour single dose
GLP:	No
Year:	1968
Species/Strain:	Rabbit (not specified)
Sex:	Male and female
No. Of Animals Per Sex Per Dose:	2
Vehicle:	None
Route Of Administration:	Neat material was applied to closely clipped intact abdominal skin under rubber dental damming secured with gauze and tape for 24 hours.
Time Of Observation Period:	14 days
Doses Administered:	4460 mg/kg as neat material, as received
LD50:	> 4460 mg/kg
Conclusions:	Moderate erythema was observed which subsided within 4 days. No eschar was observed.
Reliability:	3
Reference:	Stuaffer Chemical Company (1968) Toxicology Lab Report T-1233 Benzene Phosphinic Acid
Remarks:	None
Additional References for Acute Dermal Toxicity Studies:	None

5.1.3. Irritation

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	Draize (Federal Hazardous Substance Act 21 CFR 191.11)
Type:	Occluded, normal and abraded
GLP:	No
Year:	1968
Species/Strain:	Rabbit (not specified)
Sex:	Male and female
No. Of Animals Per Sex Per Dose:	1 male and 5 females
Vehicle:	None
Route Of Administration:	Neat material was applied to closely clipped intact abdominal skin under rubber dental damming secured with gauze and tape for 24 hours.

Time Of Observation Period:	14 days
Concentration Of Test Material:	500 mg administered neat, as received
Results:	Results: Intact skin: Erythema at 24 hours in all animals (2 had a score of 1, the remaining had a score of 2)and 2 of 6 animals had erythema scores of 1 at 48 hours. No edema was noted in at the intact administration sites. Abraded skin: All rabbits had erythema scores of 4 at 24 and 72 hours. Edema scores at 24 hours ranged from 1-3 with an average of 1.8. At 72 hours, the average erythema score as 3.7.
Conclusions:	Overall, the primary irritation index was 3.9 and considered a moderate skin irritant. Because the primary irritation index was < 5, BPA was not considered to be a primary skin irritant.
Reliability:	3
Reference:	Stuaffer Chemical Company (1968) Toxicology Lab Report T-1233 Benzene Phosphinic Acid
Remarks:	It is probable that these results are at least partially artifactual in that the material was applied as neat material. The material applied to the abraded skin was in contact with aqueous serosanguinious fluid and probably rapidly became a saturated acid solution with a pH of approximately 1. The minimal moisture at the intact sites probably lead to a lack of a significant amount of the saturated solution in contact with the skin. Contemporary practice would include wetting the material with a solvent or water to increase skin contact. If this procedure had been in this study, the response on intact and abraded skin would probably have been similar and the conclusion reached that BPA was a moderate skin irritant.
Additional References for Acute Dermal Irritation Studies:	None

5.1.4. Sensitization

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available

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Species/Strain:	No data available
Sex:	No data available
No. Of Animals Per Sex Per Dose:	No data available
Vehicle:	No data available
Route Of Administration:	No data available
Time Of Observation Period:	No data available
Concentration Of Test Material:	No data available
Results:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Acute Dermal Sensitization Studies:	None

5.1.5. Eye Irritation

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	Draize
Type:	No
GLP:	No
Year:	1968
Species/Strain:	Rabbit (not specified)
Sex:	Male and female
No. Of Animals Per Sex Per Dose:	3
Vehicle:	None
Route Of Administration:	Conjunctival sac (assumed)
Time Of Observation Period:	72 hours
Concentration Of Test Material:	10 mg of BPA as received, probably > 95%
Results:	Pain, complete destruction of eye structure and most of conjunctivia, severe hemorrhage.
Conclusions:	Severe eye irritant
Reliability:	3

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Reference:	Stuaffer Chemical Company (1968) Toxicology Lab Report T-1233 Benzene Phosphinic Acid
Remarks:	None
Additional References for Acute Eye Irritation Studies:	None

5.2. Repeated Dose Toxicity:

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Species/Strain:	No data available
Sex:	No data available
No. Of Animals Per Sex Per Dose:	No data available
Vehicle:	No data available
Route of Administration:	No data available
Time of Observation Period:	No data available
Doses Administered:	No data available
Frequency of Treatment:	No data available
NOAEL (NOEL):	No data available
LOAEL (LOEL):	No data available
Toxic Response By Dose Level:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Repeated Dose Toxicity Studies:	Haskall Laboratories (1982) Summary of Basic Toxicity 82-0083 Phenylphosphinic acid. Cited in MicroficheOTS 05555311 (1992) Eastman Kodak Co, TSCA 8e submission

5.3. Reproductive Toxicity:

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	No data available
Type:	No data available

GLP:	No data available
Year:	No data available
Species/Strain:	No data available
Sex:	No data available
No. Of Animals Per Sex Per Dose:	No data available
Vehicle:	No data available
Route Of Administration:	No data available
Time Of Observation Period:	No data available
Doses Administered:	No data available
Frequency Of Treatment:	No data available
Premating Exposure For Males:	No data available
Premating Exposure For Females:	No data available
P NOAEL (NOEL):	No data available
P LOAEL (LOEL):	No data available
F1 NOAEL (NOEL):	No data available
F1 LOAEL (LOEL);	No data available
F2 NOAEL (NOEL):	No data available
F2 LOAEL (LOEL):	No data available
P/F1/F2 Toxic Response By Dose Level:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Reproductive Toxicity Studies:	None

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5.4. *Genetic Toxicity:*

5.4.1. *In Vitro* Gene Mutations

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Cell Type:	No data available
Metabolic Activation:	No data available
Concentrations Tested:	No data available
Vehicle:	No data available
Cytotoxic Concentration:	No data available
Genotoxic Effects With Metabolic Activation:	No data available
Genotoxic Effects Without Metabolic Activation:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for In Vitro Gene Mutation Studies:	None

5.4.2. *In Vitro* Chromosome Aberrations

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Cell Type:	No data available
Metabolic Activation	No data available
Concentrations Tested:	No data available
Vehicle:	No data available
Cytotoxic Concentration:	No data available

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Genotoxic Effects With Metabolic Activation:	No data available
Genotoxic Effects Without Metabolic Activation:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for *In Vitro* Chromosome Aberration Studies:	None

5.4.3. *In Vivo* Chromosome Aberrations

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	No data available
Type:	No data available
GLP:	No data available
No data available Year:	No data available
Species/Strain:	No data available
Sex:	No data available
Route Of Administration:	No data available
Vehicle:	No data available
Doses Administered:	No data available
Genotoxic Effects:	No data available
NOAEL (NOEL):	No data available
LOAEL (LOEL):	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for *In Vivo* Chromosome Aberration Studies:	None

5.5. Developmental Toxicity:

Identity:	BPA (phosphinic acid, phenyl-) CAS# 1779-48-2
Method:	No data available
Type:	No data available

GLP:	No data available
Year:	No data available
Species/Strain:	No data available
Sex:	V
No. Of Animals Per Sex Per Dose:	No data available
Vehicle:	No data available
Route Of Administration:	No data available
Time Of Observation Period:	No data available
Doses Administered:	No data available
Frequency Of Treatment:	No data available
Maternal NOAEL (NOEL):	No data available
Maternal LOAEL (LOEL):	No data available
Fetal NOAEL (NOEL):	No data available
Fetal LOAEL (LOEL):	No data available
Maternal Toxic Response By Dose Level:	No data available
Fetal Toxic Response By Dose Level:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Developmental Toxicity Studies:	None

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BPD/BPA Coalition

BPD/BPA Coalition

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PPOA (Phenylphosphonic Acid) Robust Summaries

Submitted to the U.S. Environmental Protection Agency

by the

BPD/BPA Coalition

November, 2003

20031119080600.

1850 M Street, NW, Suite 700, Washington, DC 20036
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1. Substance Information

CAS Number:	1571-33-1
Chemical Name:	Phosphonic acid, phenyl-
Structural Formula:	$C_6H_7O_3P$
Other Names:	PPOA, phenylphosphonic acid
Exposure Limits:	Not established

2. Physical – Chemical Properties

2.1. *Melting Point:*

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	No data available
GLP:	No
Year:	No data available
Value:	162 °C
Decomposition:	No data available
Conclusions:	The melting point of PPOA is 162 °C
Reliability:	3
Reference:	Sigma-Aldrich (2002) MSDS Phenylphosphonic Acid.
Remarks:	None
Additional References for Melting Point Studies:	None

2.2. *Boiling Point:*

Identity:	PPOA
Method:	No data available
GLP:	No
Year:	No data available
Value:	Decomposes @ 271 °C
Pressure:	No data available
Pressure Unit:	No data available
Decomposition:	Decomposes @ 271 °C
Conclusions:	No boiling point because PPOA decomposes @ 271 °C
Reliability:	3
Reference:	Akzo Nobel Functional Chemicals LLC (2001) MSDS

	Phenylphosphonic Acid
Remarks:	None
Additional References for Boiling Point Studies:	None

2.3. Density:

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	No data available
GLP:	No data available
Year:	No data available
Value:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Density Studies:	None

2.4. Vapor Pressure:

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	No data available
GLP:	No
Year:	No data available
Value:	0.2 mmHg
Temperature° C:	25 °C
Pressure Unit:	mmHg
Decomposition:	No data available
Conclusions:	The vapor pressure of PPOA is 0.2 mmHg
Reliability:	3
Reference:	Akzo Nobel Functional Chemicals LLC (2001) MSDS Phenylphosphonic Acid
Remarks:	None
Additional Reference for Vapor Pressure Studies:	None

2.5. Partition Coefficient (log Kow):

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	Model calculation
GLP:	No
Year:	2003

Log Kow:	0.52
Temperature°C:	No data available
Conclusions:	The log Kow of PPOA is estimated to be 0.52
Reliability:	1
Reference:	WSKOW version 1.40
Remarks:	None
Additional References for Partition Coefficient Studies:	None

2.6. Water Solubility:

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	No data available
GLP:	No
Year:	No data available
Value at temperature°C:	278,000 mg/L
Description of solubility:	No data available
PH value and concentration at temperature °C:	No data available
Pka value at 25°C:	1.85
Conclusions:	The water soluability of PPOA is 278,000 mg/L
Reliability:	3
Reference:	Akzo Nobel Functional Chemicals LLC (2001) MSDS Phenylphosphonic Acid
Remarks:	None
Additional References for Water Solubility Studies:	PKa reference: Morelli, J.J. (2003)

2.7. Flash Point:

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	No data available
GLP:	No data available
Year:	No data available
Results:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None

Additional References for Flash Point Studies:	None

2.8. Flammability:

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	No data available
GLP:	No data available
Year:	No data available
Results:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Flammability Studies:	None

3. Environmental Fate

3.1. Photodegradation:

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	EPIWIN Model calculation: (AopWin v1.90)
GLP:	No
Type:	Model calculation
Year:	2003
Light Source:	No data available
Light Spectrum (nm):	No data available
Half-life:	57.6 hours (4.8 days for 12 hour days)
Breakdown Products:	No data available
Conclusions:	The half-life of PPOA in the atmosphere is 57.6 hours (4.8 days for 12 hour days)
Reliability	1
Reference:	AOP Version 1.90
Remarks:	None
Additional References for Photodegradation Studies:	None

3.2. Stability in Water:

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	No data available
GLP:	No data available
Type:	No data available
Year:	No data available
Half-life at a specific pH:	No data available
Breakdown Products:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Stability in Water Studies:	None

3.3. Transport (Fugacity):

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	EPIWIN Model calculation STP Fugacity model
GLP:	No
Type:	Model calculation
Year:	2003
Media:	Air, Water, Soil, Sediment

Distributions:

Compartment	Released 100% to air	Release 100% to water	Release 100% to soil
Air	11.3	0.00458	0.267
Water	24.6	99.8	20.5
Soil	64.1	0.026	79.2
Sediment	0.0422	0.171	0.0351

Adsorption Coefficient:	No data available
Desorption:	No data available
Volatility:	No data available
Conclusions:	Partitions primarily to soil and water
Reliability:	1
Reference:	EPIWIN (version 3.1) STP Fugacity model
Remarks:	When released equally to air, water, and soil, BPA is estimated to be distributed 2.92 percent to air, 46.9 percent to water, 50.1 percent to soil, and 0.0805 percent to sediment

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Additional References for Transport (Fugacity) Studies:	None

3.4. Biodegradation:

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	EPIWIN 3.10 (BIOWIN v4.00)
Type:	Model calculation
GLP:	No
Year:	2003
Degradation% after time:	No data available
Breakdown Products:	No data available
Concentration Of Test Chemical:	No data available
Analytical Method:	No applicable
Conclusions:	Ultimate Biodegradation Timeframe: weeks Primary Biodegradation Timeframe: days-weeks
Reliability:	1
Reference:	BIOWIN Version 4.00
Remarks:	None
Additional References for Biodegradation Studies:	None

3.5. Bioconcentration:

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	EPIWIN 3.10 (Bcfwin v2.14)
Type:	Model calculation
GLP:	No
Year:	2003
Results:	Log BCF = 0.5 (BCF = 3.162)
Conclusions:	Not expected to bioaccumulate
Reliability:	1
Reference:	Bcfwin Version 2.14
Remarks:	None
Additional References for Bioconcentration Studies:	None

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4. Ecotoxicity

4.1. Acute Toxicity to Fish:

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	EPIWIN 3.10 (ECOSAR Version 0.99)
Type:	Model calculation
GLP:	No
Year:	2003
Species/Strain/:	Not applicable
Supplier:	Not applicable
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Nominal/Measured Concentrations:	Not applicable
LC50:	28848.1 mg/L
Conclusions:	Predicted to be practically nontoxic to fish
Reliability:	1
Reference:	ECOSAR Version 0.99
Remarks:	None
Additional References for Acute Toxicity to Fish Studies:	None

4.2. Acute Toxicity to Invertebrates:.

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	EPIWIN 3.10 (ECOSAR version 0.99)
Type:	Model calculation
GLP:	No
Year:	2003
Species/Strain/:	Daphnid
Supplier:	Not applicable
Analytical Monitoring:	No applicable
Exposure Period:	48 hours
Nominal/Measured Concentrations:	Not applicable
LC50:	27907.3 mg/L
Conclusions:	Predicted to be practically nontoxic to invertebrates
Reliability:	1
Reference:	ECOSAR version 0.99
Remarks:	None

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Additional References for Acute Toxicity to Invertebrates Studies:	None

4.3. Acute Toxicity to Aquatic Plants:

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	EPIWIN 3.10 (ECOSAR version 0.99)
Type:	Model calculation
GLP:	No
Year:	2003
Species/Strain/ Supplier:	Green algae
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Nominal/Measured Concentrations:	Not applicable
EC50:	3829.8 mg/L
Conclusions:	Predicted to be practically non toxic to green algae
Reliability:	1
Reference:	ECOSAR version 0.99
Remarks:	None
Additional References for Acute Toxicity to Aquatic Plants Studies:	None

5. Mammalian Toxicity

5.1. Acute Toxicity:

5.1.1. Oral

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	OPPTS 870.110
Type:	Guideline
GLP:	Yes
Year:	2000
Species/Strain:	Rat / Crl:CD(SD)IGS BR
Sex:	Male and female
No. Of Animals Per Sex Per Dose:	10
Vehicle:	Distilled water

Route Of Administration:	Oral gavage
Time Of Observation Period:	14 days
Doses Administered:	500 or 2000 mg/kg (dose volume: 5 mL/kg)
LD50:	Between 500 and 2000 mg/kg
Conclusions:	At 500 mg/kg, the clinical sign of staggered gait was seen in 4 of 10 males and 3 of 10 females on the day of dosing. These signs resolved and the animals appeared normal throughout the study and gained body weight. At 2000 mg/kg 3 of 10 males and 4 of 10 females died within 2 days of dosing. Clinical signs included hypoactivity, staggered gait, flaccidity, tremors, liquid feces, and thin appearance. Necropsy observations included multiple dark brown indistinct areas or multiple black eroded areas in the glandular mucosa of the stomach. In two animals the glandular mucosa was thickened and the omentum was dark red and gelatinous.
Reliability:	1
Reference:	Akzo Nobel Chemicals, Inc. (2000) Covance Study 00502647 Acute Oral Toxicity of Phenyl Phosphonic Acid (PPOA) in Rats
Remarks:	The clinical signs and necropsy findings are consistent with the interpretation of effects of ingestion of a strong acid and acute injury to the gastrointestinal tract.
Additional References for Acute Oral Toxicity Studies:	Stuaffer Chemical Company (1972) Toxicology Lab Report T-1918 Benzene Phosphonic Acid

5.1.2. Dermal

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	EPA/OECD Guidelines
Type:	Guideline
GLP:	Yes
Year:	200
Species/Strain:	Rat / Crl:CD(SD)IGS BR
Sex:	Male and Female
No. Of Animals Per Sex Per Dose:	5
Vehicle:	Distilled water
Route Of	Occlusive patch covering gauze with moistened test article

Administration:	
Time Of Observation Period:	14
Doses Administered:	2000 mg/kg to an area of approximately 20 cm^2
LD50:	> 2000 mg/kg
Conclusions:	No mortality and all animals gained weight throughout the study. Maximum individual animal erythema scores ranged from slight to severe. Maximal individual edema reactions ranged from slight to moderate. Subcutaneous hemorrhaging was observed in 2 animals, necrotic appearing areas in another, and fissuring in another. The observed irritation cleared in all 10 animals by the Day 14 observation.
Reliability:	1
Reference:	Akzo Nobel Chemicals Inc. (2000) Covance Study Number 00502648. Acute Dermal Toxicity Study of Phenyl Phosphonic Aid (PPOA) in Rats
Remarks:	None
Additional References for Acute Dermal Toxicity Studies:	Stuaffer Chemical Company (1972) Toxicology Lab Report T-1918 Benzene Phosphonic Acid

5.1.3. Irritation

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	OPPTS 870.2500
Type:	Guideline
GLP:	Yes
Year:	2000
Species/Strain:	Rabbits / Hra(NZW)SPF
Sex:	Male and female
No. Of Animals Per Sex Per Dose:	Two male and one female
Vehicle:	Distilled water
Route Of Administration:	Semioccclusive patch for 4 hours
Time Of Observation Period:	7 days
Concentration Of Test Material:	500 mg, neat, as received
Results:	Severe erythema dnd slight to moderate edema reactions were observed. Necrotic appearing areas and skin

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	ulcerations were observed at all three test sites. Ulceration of the skin at the test site of all three animals prompted termination of the study on Day 7. The primary dermal irritation index was 6.5 corresponding to a classification of "severely irritating"
Conclusions:	The material was considered to be severely irritating to rabbit skin
Reliability:	1
Reference:	Akzo Nobel Chemicals Inc. (2000) Covance Study Number 00502649. Primary Dermal Irritation/Corrosion Study of Phenyl Phosphonic Acid (PPOA) in Rabbits
Remarks:	None
Additional References for Acute Dermal Irritation Studies:	None

5.1.4. Sensitization

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	OPPTS 870.2600
Type:	Guideline
GLP:	Yes
Year:	2000
Species/Strain:	Guinea pig / Crl(HA) BR
Sex:	Male
No. Of Animals Per Sex Per Dose:	20 in the Test Group and 10 in the Irritation Control Group
Vehicle:	Mineral oil (for the test material for the intradermal injection on Day 1) Petrolatum (for the test material in the topical induction phase and the challenge phase)
Route Of Administration:	Intradermal and topical
Time Of Observation Period:	24 days
Concentration Of Test Material:	Intradermal 1% w/v in mineral oil Topical induction: 50% w/w in petrolatum Challenge: 10% w/w in petrolatum
Results:	None of the animals in the test or irritation control groups exhibited a dermal reaction to the challenge applications of the test or control materials.
Conclusions:	Because no animals were considered to have exhibited sensitizations reactions, the criterion in the EU guideline of

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	30% was not met, and PPOA is not considered a sensitizer.
Reliability:	4
Reference:	Akzo Nobel Chemicals Inc. (2000) Covance Sturdy Number 00502651. Dermal Sensitization on Phenyl Phosphonic Acid (PPOA) In Guinea Pigs –Maximization Test
Remarks:	Because PPOA moistened with water is severely irritating, the lack of irritation in the irritation screening study calls into questions the extent of PPOA exposure when applied in petrolateum.
Additional References for Acute Dermal Sensitization Studies:	None

5.1.5. Eye Irritation

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	CFR 191.12
Type:	Guideline
GLP:	No
Year:	1972
Species/Strain:	New Zealand rabbits
Sex:	No data available
No. Of Animals Per Sex Per Dose:	No data available
Vehicle:	None
Route Of Administration:	Conjunctival sac
Time Of Observation Period:	24, 48, and 72 hours
Concentration Of Test Material:	10 mg of neat PPOA
Results:	All test rabbits exhibited gross destruction of the cornea and all surrounding tissues
Conclusions:	Corrosive
Reliability:	2
Reference:	Stauffer Chemical Company (1972) Toxicology Lab Report T-1918. Benzene Phosphonic Acid
Remarks:	None
Additional References for Acute Eye Irritation Studies:	None

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5.2. Repeated Dose Toxicity:

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Species/Strain:	No data available
Sex:	No data available
No. Of Animals Per Sex Per Dose:	No data available
Vehicle:	No data available
Route of Administration:	No data available
Time of Observation Period:	No data available
Doses Administered:	No data available
Frequency of Treatment:	No data available
NOAEL (NOEL):	No data available
LOAEL (LOEL):	No data available
Toxic Response By Dose Level:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Repeated Dose Toxicity Studies:	None

5.3. Reproductive Toxicity:

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Species/Strain:	No data available
Sex:	No data available
No. Of Animals Per Sex Per Dose:	No data available
Vehicle:	No data available
Route Of	No data available

Administration:	
Time Of Observation Period:	No data available
Doses Administered:	No data available
Frequency Of Treatment:	No data available
Premating Exposure For Males:	No data available
Premating Exposure For Females:	No data available
P NOAEL (NOEL):	No data available
P LOAEL (LOEL):	No data available
F1 NOAEL (NOEL):	No data available
F1 LOAEL (LOEL);	No data available
F2 NOAEL (NOEL):	No data available
F2 LOAEL (LOEL):	No data available
P/F1/F2 Toxic Response By Dose Level:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Reproductive Toxicity Studies:	None

5.4. *Genetic Toxicity:*

5.4.1. *In Vitro* Gene Mutations

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	OECD 409
Type:	Guideline
GLP:	Yes
Year:	2000

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Cell Type:	TA98, TA100, TA1535, TA1537 and WP2*uvr*A
Metabolic Activation:	S9 homogenate prepared from male Sprague-Dawley rats that that been dosed with Aroclor 1254
Concentrations Tested:	33.3, 100, 333, 1000, 3330, and 5000 µg plate
Vehicle:	DMSO
Cytotoxic Concentration:	In the definitive study, there were indications of cytotoxicity for the *e. Coli* strains at 3330 µg plate and all cell types tested at 5000 µg plate.
Genotoxic Effects With Metabolic Activation:	None observed
Genotoxic Effects Without Metabolic Activation:	None observed
Conclusions:	Not genotoxic in the test systems used
Reliability:	2
Reference:	Akzo Nobel Chemicals, Inc. (2000) Covance Study Number 21552-0-409OECD. Salmonella-Escherichia coli/Mammalian-Microsome Reverse Mutation Assay with a Confirmatory Assay with Phenyl Phosphonic Acid (PPOA)
Remarks:	None
Additional References for In Vitro Gene Mutation Studies:	None

5.4.2. *In Vitro* Chromosome Aberrations

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Cell Type:	No data available
Metabolic Activation	No data available
Concentrations Tested:	No data available
Vehicle:	No data available
Cytotoxic Concentration:	No data available
Genotoxic Effects With Metabolic Activation:	No data available
Genotoxic Effects	No data available

Without Metabolic Activation:	
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for *In Vitro* Chromosome Aberration Studies:	None

5.4.3. *In Vivo* Chromosome Aberrations

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Species/Strain:	No data available
Sex:	No data available
Route Of Administration:	No data available
Vehicle:	No data available
Doses Administered:	No data available
Genotoxic Effects:	No data available
NOAEL (NOEL):	No data available
LOAEL (LOEL):	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for *In Vivo* Chromosome Aberration Studies:	None

5.5. Developmental Toxicity:

Identity:	PPOA (phosphonic acid, phenyl-) CAS# 1571-33-1
Method:	No data available
Type:	No data available
GLP:	No data available
Year:	No data available
Species/Strain:	No data available
Sex:	No data available
No. Of Animals Per	No data available

Sex Per Dose:	
Vehicle:	No data available
Route Of Administration:	No data available
Time Of Observation Period:	No data available
Doses Administered:	No data available
Frequency Of Treatment:	No data available
Maternal NOAEL (NOEL):	No data available
Maternal LOAEL (LOEL):	No data available
Fetal NOAEL (NOEL):	No data available
Fetal LOAEL (LOEL):	No data available
Maternal Toxic Response By Dose Level:	No data available
Fetal Toxic Response By Dose Level:	No data available
Conclusions:	No data available
Reliability:	No data available
Reference:	No data available
Remarks:	None
Additional References for Developmental Toxicity Studies:	None

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