FOREWORD INTRODUCTION

1,3-PENTADIENE

CAS N°:504-60-9

Substance

End Point	:	**IDENTIFIERS, PHYSICAL AND CHEMICAL PROPERTIES**
Chemical Name	:	**1,3-Pentadiene**
Common Name	:	**1,3-Pentadiene**
CAS Number	:	**504-60-9**
RTECS Number	:	**RZ2464000**

Synonyms

Methyl butadiene
1-Methylbutadiene
Piperylene
1,3-PD

Properties & Definitions

Molecular Formula	:	**C5H8**
Molecular Weight	:	**68**
Melting Point	:	**-87C(trans) ***
Boiling Point	:	**42C(trans), 44C(cis)**
State	:	**Liquid**
Flash Point	:	**-28C (c-cup)**
Flamable Limit	:	**Flammable**
Density	:	**0.68 (trans), 0.69 (cis)**
Vapour Pressure	:	**53.3 kPa at 25C (trans)**
Octanol/Water Partition Coefficient	:	**log Pow = 1.5 (estimated)**
Water Solubility	:	**690 mg/L (estimated)**
Solubility in other Solvents	:	**Soluble in Ether, Alcohol, Acetone, Benzene**
Colour	:	**Colourless**
Additives	:	**2,6-di-tert-butylene-p-cresol (BHT); tert-butyl catechol**
Impurities	:	**Cyclopentene; 2-methyl-2-butene**
Definitions	:	**This chemical has trans and cis isomers which have CAS Numbers of 2004-70-8 and 1574-41-0 respectively. CAS Number 504-60-9 is for unspecified or mixed isomer.**
General Comments	:	Piperylene can undergo polymerisation. Index of refraction:1.43 (trans), 1.43 (cis). Lowest explosivity: 2% (trans), 2% (cis). Purity of industrial product: 30-80%. * MP (cis): -141C.

Overall Evaluation

SIDS INITIAL ASSESSMENT

PRESENTLY OF LOW PRIORITY FOR FURTHER WORK

1,3-pentadiene (1,3-PD) is handled in close sysems at a limited number of sites as an intermediate in the manufacture of C5 hydrocarbon or petroleum resins. Potential exposures to 1,3-PD are limited to the workplace where inhalation would be the primary route of exposure. Workplace exposure is estimated to be low, below 1 ppm, 8-hour TWA.

1,3-PD is not expected to cause significant environmental effects. As a very volatile chemical, the main exposure route to 1,3-PD is inhalation. 1,3-PD is expected to volatilize rapidly from various media (water, soil). 1,3-PD can undergo photo-oxidation with a short half live of less than several hours. It is not expected to appreciably bioconcentrate in aquatic species based on a calculated Log Pow of 2.43. Acute toxicity studies in fish (fathead minnows), invertebrates (daphnids) and algae indicate a low environmental concern.

No adverse effects have been reported in humans exposed to 1,3-PD. 1,3-PD has been studied in a number of animal studies. It displayed a low order of acute toxicity (oral, dermal, inhalation) in rats and/or rabbits. It was non-genotoxic in two in vitro assays; Ames and mouse lymphoma mutation assay. By the inhalation route, 1,3-

PD was inactive in a micronucleus study in rats (7000 ppm) and mice (300 ppm) at the highest dose (est. MTD) tested. In an oral screening study in rats at a dose up to 1 g/kg, 1,3-PD did not produce evidence of systemic lesions, reproductive toxicity, and developmental toxicity. The findings on 1,3-PD were very comparable with isoprene, an isomer of 1,3-PD. A review of the available health effects data (animal, man) indicate a low order of health concern for 1,3-PD.

1-3-PD has been used in a safe manner for a number of years. The lack of adverse effects in man may be due to low exposure to 1,3-PD and low order of toxicity of 1,3-PD in various tests. 1,3-PD has not produced any adverse effects in the environment which may be due to low exposure and low order of toxicity of 1,3-PD in various tests.

EXPOSURE

GENERAL DISCUSSION

The limited data for this enclosed intermediate which is used in the manufacture of C5 hydrocarbon or petroleum resins indicates a low exposure to the environment, consumers and the workplace.

ENVIRONMENTAL EXPOSURE

Based on its current use, there is expected to be low environmental exposure to 1,3-PD.

CONSUMER EXPOSURE

Based on its current use, there is expected to be low exposure to 1,3-PD.

WORKPLACE EXPOSURE

Some limited data indicates low exposure, less than 1 ppm 8-hour TWA.

TOXICITY

HUMAN TOXICITY

No adverse effects have been reported in humans exposed to 1,3-PD.

ANIMAL TOXICITY

1,3-PD displayed a low order of acute toxicity; oral, dermal and inhalation. It was non-genotoxic in two in vitro assays: Ames and mouse lymphoma mutation assay. In addition, it was inactive in a in vivo genotoxic assay (micronucleus assay) in rats and mice by the inhalation route. In an oral screening study in rats, 1,3-PD displayed no systemic lesions, reproductive effects or developmental effects with the NOAEL being 1000 mg/kg, the highest dose tested.

ECOTOXICITY

1,3-PD displayed a low order of acute toxicity in fish (fathead minnow), invertebrates (daphnids) and algae. Based on its physical and chemical properties, the material is not expected to be hydrolyzed, will readily be vaporized from various media (soil, water), will readily undergo photooxidation, and will not persist in the environment.

CONCLUSIONS

Based on use considerations and health and environmental data, we conclude that 1,3-PD falls into the category of "presently of low concern".

RECOMMENDATIONS

Based on existing data on 1,3-PD, no further studies (health, environmental) would seem warranted for 1,3-PD.

Production-Trade

Chemical Name	:	**1,3-Pentadiene**
CAS Number	:	**504-60-9**
Geographic Area	:	**USA**

Production

Quantity	*Year*
4990-27670 t - P	**1977**
4536-22680 t - P	**1982**

General Comments : The public portion of the TSCA Inventory (1982) reports 1977 U.S. production of 11-61 million pounds (4990-27670 t) of 1,3-pentadiene and 1 to 10 million pounds of trans-1,3-pentadiene. At least 10 to 50 million pounds (4536-22680 t) per year of 1,3-pentadiene are produced. Du Pont (1982), the only known major producer of trans-1,3-pentadiene, reported annual production of trans-1,3-pentadiene at 200000 to 1 million pounds. The following references are also cited: TSCA Inventory (1982) TSCA Inventory of Producers of Chemicals in Commerce for 1977. Washington, DC U.S. EPA.

References

!SIDSP*
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

CRCPR*
CRC Inc. Preliminary Information Review (Working Draft), (1982)

Uses

Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**

Use

Quantity	*Year*	*Comments*
		1,3-Pentadiene is primarily used as a monomer in a closed system for the industrial manufacture of C5 resins.

References

Primary References : **CRCPR***
CRC Inc. Preliminary Information Review (Working Draft), (1982)

Secondary References : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point	:	**HUMAN INTAKE AND EXPOSURE**
Chemical Name	:	**1,3-Pentadiene**
CAS Number	:	**504-60-9**

Test Subject

Organism	*Medium*	*Specification*	*Route*	*Lifestage*	*Sex*
HUMAN					

Test Results

General Comments : The potential worker exposure to 1,3-PD during customer use apparently refers to exposure during manufacture of C5 aliphatic resins. Workers coming into contact with the uncured resin in industrial applications (e.g., in the tire industry) as well as workers exposed to cured resins containning any residual monomer, are also potentially exposed to 1,3-PD compound.

References

Primary Reference : **CRCPR***
CRC Inc. Preliminary Information Review (Working Draft), (1982)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point	:	**BIODEGRADATION**
Chemical Name	:	**1,3-Pentadiene**
CAS Number	:	**504-60-9**
Study type	:	**LAB**

Test Subject

Organism	*Medium*	*Specification*
	AQ	**SLUDG**

Species/strain/system : 1,3-PD was incubated with an unacclimated sewage seed inoculum.

Test Method and Conditions

Test method description : OECD 301 D; GLP: yes. Test result is based on dissolved oxygen loss. 1,3-PD was tested in a closed bottle system due to its volatility.

(An)aerobic : **AEROB**

Test Results

Quantity	*Time*	*Comments on result*
2.5 %	**28 d**	2.5% biodegradation in 28 days.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 91 MRL 280, (1991)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point	:	**PHOTODEGRADATION**
Chemical Name	:	**1,3-Pentadiene**
CAS Number	:	**504-60-9**

Evaluations

Evaluation text	:	Like other diolefins, 1,3-PD is expected to undergo photo oxidation with a half-life of several hours or less. The following references are also cited: CRCS. Inc. (1982) Preliminary Information Review (Working Draft) for 1,3- Pentadiene. 14 pages; Howard, P. H. (1990) Handbook of environmental fate and exposure data for organic chemicals. Volume 1, 1,3-Butadiene p. 101-106. Editor P. H. Howard, Lewis Publishers.

References

Primary Reference	:	**ESTHAG** Darnall, K. R. et al. Environmental Science and Technology, 10(7), 692-696, (1976)
Secondary Reference	:	**!SIDSP*** OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point	:	**HYDROLYSIS**
Chemical Name	:	**1,3-Pentadiene**
CAS Number	:	**504-60-9**

Evaluations

Evaluation text	:	1,3-Pentadiene is not expected to undergo hydrolysis in water. The following references are also cited: CRCS. Inc. (1982) Preliminary Information Review (Working Draft) for 1,3-Pentadiene. 14 pages; Howard, P.H. (1990) Handbook of environmental fate and exposure data for organic chemicals. Volume 1, 1,3-Butadiene, p. 101-106. Editor P.H. Howard, Lewis Publishers.

References

Primary Reference	:	**ESTHAG** Darnall, K. R. et al. Environmental Science and Technology, 10(7), 692-696, (1976)
Secondary Reference	:	**!SIDSP*** OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point	:	**ABSORPTION**
Chemical Name	:	**1,3-Pentadiene**
CAS Number	:	**504-60-9**

Evaluations

Evaluation text : No data are available for toxicodynamics nor toxico-kinetics. Like other diolefins such as isoprene, 1,3-pentadiene is likely to be absorbed.

References

Secondary Reference :

!SIDSP*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point	:	**BIOCONCENTRATION**
Chemical Name	:	**1,3-Pentadiene**
CAS Number	:	**504-60-9**

Evaluations

Evaluation text	:	A low octanol/water partition coefficient suggests a low degree of bioaccumulation or biomagnification.

References

Primary Reference	:	**CRCPR*** CRC Inc. Preliminary Information Review (Working Draft), (1982)
Secondary Reference	:	**!SIDSP*** OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point	:	**METABOLISM**
Chemical Name	:	**1,3-Pentadiene**
CAS Number	:	**504-60-9**

Evaluations

Evaluation text	:	No data are available for toxicodynamics nor toxico-kinetics. Like other diolefins such as isoprene, 1,3-pentadiene is likely to be metabolized. Mice are predicted to metabolize 1,3-PD more efficiently than rats.

References

Secondary Reference	:	**!SIDSP*** OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **MAMMALIAN ACUTE TOXICITY**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**

Species/strain/system : Sprague-Dawley rats
Exposure Period : **4 h**
Dose / Concentration : **20917 ppm**

Test Method and Conditions

Test method description : OECD 403 4-hour exposure; GLP: yes

Test Results

Organism	Medium	Spec.	Route	Lifestage	Sex	Effect	Effect Comments
RAT			**IHL**	**6wk**	**M F**	**LC50**	LC50 for 4 hours is greater than 20917 ppm equivalent to 58.2 mg/L.

General Comments : This finding is in agreement with predicted values and known health effects data on 1,3-pentadiene, technical grade 1,3-pentadiene and other diolefins. The following reference is also cited: shugaev, B.B. et al. (1979) Biofizika 24 (1), 160-162. Exposure comments: A target concentration was 55.6 mg/L (20000 ppm) and the actual mean concentration was 58.2 mg/L (20917 ppm) with a standard deviation of 0.85 mg/L (307.2 ppm).

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 91 MRL 212, (1991)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **MAMMALIAN ACUTE TOXICITY**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**

Species/strain/system : B6C3F1 mice
Exposure Period : **4 h**
Dose / Concentration : **20917 ppm**
Exposure comments : A target concentration 55.6 mg/L (20000 ppm) and the actual mean concentration was 58.2 mg/L (20917 ppm) with a standard deviation of 0.85 mg/L (307.2 ppm).

Test Method and Conditions

Test method description : OECD 403 4-hour exposure; GLP: yes

Test Results

Organism	*Medium*	*Spec.*	*Route*	*Lifestage*	*Sex*	*Effect*	*Effect Comments*
MOUSE			**IHL**	**6-9wk**	**M** **F**	**LC50**	LC50 for 4 hours is less than 20917 ppm equivalent to 58.2 mg/L. All the mice were dead by the end of the second hour of exposure.

General Comments : This finding is in agreement with predicted values and known health effects data on 1,3-pentadiene, technical grade 1,3-PD and other diolefins. Other report says that 2 hours LC50 for the cis and trans isomer were 16200 ppm and 1440 ppm, respectively. The following reference is also cited: Shugaev,B.B. et al.(1979) Biofiyika 24 (1), 160-162.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 91 MRL 212, (1991)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **MAMMALIAN ACUTE TOXICITY**
Chemical Name : **1.3-Pentadiene**
CAS Number : **504-60-9**

Species/strain/system : New Zealand rabbits
Exposure Period : **24 h**
Dose / Concentration : **3160 mg/kg BW**
Exposure comments : The test material was applied as a single dose to not less than 10% of the body surface.

Test Method and Conditions

Test method description : OECD 402; GLP: yes

Test Results

Organism	*Medium*	*Spec.*	*Route*	*Lifestage*	*Sex*	*Effect*	*Effect Comments*
RBT			**SKN**	**15wk** **15wk**	**M** **F**	**LD50**	LD50 for 24 hours is greater than 3.2 g/kg. No death at a limit dose of 3.2 g/kg.

General Comments : This finding is in agreement with the predicted findings and data on piperylene concentrate, and related diolefins. Hence, 1,3-pentadiene displays a low order of toxicity by the dermal route.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 91 MRL 263, (1991)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **MAMMALIAN ACUTE TOXICITY**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**

Species/strain/system : Sprague-Dawley rats
Exposure Period : **1 X**
Dose / Concentration : **5000 mg/kg BW**

Test Method and Conditions

Test method description : OECD 401 - Limit test; GLP: yes

Test Results

Organism	Medium	Spec.	Route	Lifestage	Sex	Effect	Effect Comments
RAT			**ORL**	**8wk** **10wk**	**M** **F**	**LD50**	LD50 is less than 5000 mg/kg. Seven rats died during the study (3/5 males and 4/5 females).

General Comments : A range finding oral study for the repeated dose study of 1,3-pentadiene in Sprague-Dawley rats revealed an oral LD50 > 1 g/kg. The predicted oral LD50 is >= 2 g/kg. Another limit study (2 g/kg) may be done on 1,3-pentadiene to confirm these predictions.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 91 MRL 208, (1991)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **MAMMALIAN TOXICITY**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**

Test Subject

Organism	*Medium*	*Specification*	*Route*	*Lifestage*	*Sex*	*Number exposed*	*Number controls*
HUMAN							

Exposure

Exposure Type : **OCC**
Exposure Period : **8 h**
General Comments : No ACGIH TLV or OSHA PEL exist for 1,3-PD. A workplace environmental exposure level (WEEL) guide of 50 ppm (8 hours TWA) has been recommended for isoprene, an isomer of 1,3-PD.

References

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **MAMMALIAN TOXICITY**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**
Study type : **LAB**

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
MOUSE			**IHL**		**M**	**2**	
					F	**2**	

Test Method and Conditions

Test method description : This test was done to assist in the dose selection for the micronucleus study.

Exposure

Exposure Type : **SHORT**
Exposure Period : **2 d**
Frequency : **6 h/d**
Dose / Concentration : **100-2000 ppm**
Exposure comments : Mice were exposed 6 hours a day, for 2 days to target concentrations of 0, 100, 500 and 2000 ppm 1,3-PD equivalent to 0, 0.278, 1.39 and 5.56 mg/L.

Test Results

Organ	Effect	Rev.	OnSet	Sex	Affected in Exposed - Controls
	DEATH				

All the mice survived at 100 ppm but they all died at >= 500 ppm.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 92 MRL 36, (1992)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **MAMMALIAN TOXICITY**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**
Study type : **LAB**

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
RAT							

Species/strain/system : Sprague-Dawley rats

Test Method and Conditions

Test method description : OECD protocol on Combination Repeat Dose and Reproductive/Developmental Toxicity Screening; GLP: yes

Test Results

Organ	*Effect*	*Rev.*	*OnSet*	*Sex*	*Affected in Exposed - Controls*
WB	**NEF**				

No systemic effects observed based on gross and microscopic evaluations of organs.

NEL

Dose or concentration at which no toxic effects were observed: 1000 mg/kg (highest dose tested).

General Comments : A related diolefin (isoprene) also showed a low order of systemic toxicity in rats. Hence, the findings on 1,3-pentadiene were not unexpected. The following references are also cited: Melnick, R. L. et al. (1990) Env. Hlth. Persp. 86, 93-98; Gage, J. C. (1970) Br. J. Ind. Med. 27, 1-18.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 92 MRL 90, (1992)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point	:	**CARCINOGENICITY**
Chemical Name	:	**1,3-Pentadiene**
CAS Number	:	**504-60-9**

Evaluations

Evaluation text	:	A related isomer, isoprene did not appear to be carcinogenic in rats at an inhalation dose up to 7000 ppm.

References

Primary Reference	:	**PAACR*** Melnick, R. L. et al. Proceedings of the American Association for Cancer Research, 33, 687, (1992)
Secondary Reference	:	**!SIDSP*** OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **MUTAGENICITY**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**
Study type : **LAB**

Test Subject

Organism	*Medium*	*Specification*	*Route*	*Lifestage*	*Sex*	*Number exposed*	*Number controls*
BACT			**VTR**				

Species/strain/system : Salmonella typhimurium, 5 or 6 strains with and without metabolic activation.

Test Substance

Description of the test substance : Trans 1,3-PD (99%, CAS No. 2004-70-8), cis 1,3-PD (98%, CAS No. 1574-41-0), 1,3-PD(98%, mixed isomers, CAS No. 504-60-9)

Test Method and Conditions

Test method description : Bacterial test. OECD 471. GLP confirmed for cis 1,3-PD and 1,3-PD(mixed isomers) and not confirmed for trans 1,3-PD.

Exposure

Dose / Concentration : **32-3200 ug/ PLATE**
Exposure comments : 32-3200 ug/plate of 1,3-PD (mixed isomers) or cis 1,3-PD was applied.

Test Results

Organ	*Effect*	*Rev.*	*OnSet*	*Sex*	*Affected in Exposed - Controls*
PHENO	**NEF**				

Inactive in all tests. Minimum concentration of test substance at which toxicity to bacteria was observed: with metabolic activation; =< 2ug/plate(trans), =< 3.2 ug/plate (cis, mixed) without metabolic activation: =< 3.2 ug/plate (trans, cis and mixed).

General Comments : These tests were performed for trans 1,3-PD, cis 1,3-PD and mixed isomer of 1,3-PD respectively. These negative findings are consistent with negative findings on isoprene, an isomer of 1,3-PD. Another diolefin, 1,3-butadiene, was active in the Salmonella assay. The following references are also cited: Exxon Biomedical Sciences, Inc.(1991) 91 MRL 291; Liewen, M.B. and Martin, E. H. (1985) Mutation Research 157, 49-52; Mortelmans, K. L. et al. (1986) Env. Mutagen. 8, Suppl 7, 1-119; Arce, G. T. et al (1990) Env. Hlth. Persp. 86, 75-78.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 92 MRL 1, (1992)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **MUTAGENICITY**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**
Study type : **LAB**

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
MOUSE			**IHL**	**8-9wk**	**M**	**15/DOSE**	**15**
				8-9wk	**F**	**15/DOSE**	**15**

Species/strain/system : B6C3F1 mice

Test Method and Conditions

Test method description : Bone Marrow Micronucleus Test. OECD 474; GLP: yes

Exposure

Exposure Type : **SHORT**
Exposure Period : **2 d**
Frequency : **6 h/d**
Dose / Concentration : **30-300 ppm**
Exposure comments : The target inhalation concentrations were 30, 100 and 300 ppm equivalent to 0.083, 0.278 and 0.834 mg/L.

Test Results

Organ	Effect	Rev.	OnSet	Sex	Affected in Exposed - Controls
	NEF				

No increase in bone marrow micronucleus in mice. The highest inhalation dose was 300 ppm. No evidence of bone marrow toxicity was detected.

General Comments : The negative finding in mice (=< 300 ppm) is in agreement with negative clastogenic data on isoprene in mice at concentrations of =< 220 ppm. 1,3-Butadiene produced micronuclei effects in mice at >= 63 ppm but not at the lowest dose tested, 6 ppm. The following reference is also cited: Shelby M. D. (1990) Env. Hlth. Persp. 86, 79-84.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 92 MRL 36, (1992)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **MUTAGENICITY**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**
Study type : **LAB**

Test Subject

Organism	*Medium*	*Specification*	*Route*	*Lifestage*	*Sex*	*Number exposed*	*Number controls*
MOUSE			**VTR**				

Species/strain/system : L5178Y Mouse Lymphoma Cell

Test Substance

Description of the test substance : Cis 1,3-pentadiene (98%, CAS No. 1574-41-0)

Test Method and Conditions

Test method description : Cytogenetic analysis; GLP: yes

Test Results

Organ	*Effect*	*Rev.*	*OnSet*	*Sex*	*Affected in Exposed - Controls*
	NEF				

Inactive with and without metabolic activation. Lowest concentration producing cell toxicity; with metabolic activation; 200 ug/L, without metabolic activation; 400 ug/L

General Comments : 1,3-PD was inactive under these test conditions. Isoprene was also inactive in in vitro cytogenetic studies in CHO cells looking at SCE and chromosomal aberrations. The following reference is also cited: National Toxicology Annual Plan (1990) Fiscal Year 1990 Annual Plan, page 64.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., (1988)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **MUTAGENICITY**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**
Study type : **LAB**

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
RAT			**IHL**	**11-12wk**	**M**	**15/DOSE**	**15**
				11-12wk	**F**	**15/DOSE**	**15**

Species/strain/system : Sprague-Dawley rats

Test Method and Conditions

Test method description : Bone marrow micronucleus test. OECD 474; GLP: yes

Exposure

Exposure Type : **SHORT**
Exposure Period : **2 d**
Frequency : **6 h/d**
Dose / Concentration : **350-7000 ppm**
Exposure comments : The target inhalation concentrations were 350, 3500 and 7000 ppm equivalent to 0.973, 9.73, and 19.5 mg/L.

Test Results

Organ	Effect	Rev.	OnSet	Sex	Affected in Exposed - Controls
	NEF				

No increase in bone marrow micronucleus in rats. The highest inhalation dose was 7000 ppm equivalent to 19.5 mg/L . No evidence of bone marrow toxicity was detected.

General Comments : This negative finding was in agreement with no clastogenic effects in rats for 1,3-butadiene. The following reference is also cited: Cunningham, M. J. et al. (1986) Mutagenesis, 1, 449-452.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 92 MRL 62, (1992)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point	:	**NEUROTOXICITY**
Chemical Name	:	**1,3-Pentadiene**
CAS Number	:	**504-60-9**

Evaluations

Evaluation text	:	Subchronic oral study in rats (=< 1000 mg/kg) on 1,3-PD revealed no evidence of treatment related effects or neurotoxicity (i.e., irreversible lesions). Rats exposed to a related diolefin (isoprene) also failed to produce neuropathological lesions.

References

Primary Reference : **EVHPAZ**

Melnick, R. L. et al. Environmental Health Perspectives, DHEW Publication, 86, 93-98, (1990)

Secondary Reference : **!SIDSP***

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **IRRITATION**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**

Evaluations

Evaluation text : Based on health effects data on related analogs, 1,3-PD is not expected to be a severe eye irritant. It is unlikely to produce effects on the cornea. Eye irritation (rabbit) data exist on technical grade 1,3-PD, but its relevance to pure 1,3-PD is questionable.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 91 MRL 263, (1991)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **IRRITATION**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**
Study type : **LAB**

Test Subject

Organism	Medium	Specification	Route	Lifestage	Sex	Number exposed	Number controls
RBT			**SKN**				

Species/strain/system : New Zealand rabbits

Test Method and Conditions

Test method description : GLP: yes

Exposure

Exposure Type : **ACUTE**
Exposure Period : **24 h**

Test Results

Organ	Effect	Rev.	OnSet	Sex	Affected in Exposed - Controls
SKIN	**IRRIT**				

24-hour dermal contact with 3.2 g/kg produced moderate dermal irritation.

General Comments : The material is expected to be a mild-moderate dermal irritant depending on the test conditions.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 91 MRL 263, (1991)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **REPRODUCTION**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**
Study type : **LAB**

Test Subject

Organism	*Medium*	*Specification*	*Route*	*Lifestage*	*Sex*	*Number exposed*	*Number controls*
RAT			**ORL**				

Species/strain/system : Sprague-Dawley rats

Test Method and Conditions

Test method description : OECD on Combination Repeat Dose and Reproductive/Developmental Toxicity Screening; GLP: yes

Exposure

Dose / Concentration : **30-1000 mg/kg**
Exposure comments : Rats were given an oral dose of 30, 100 and 100 mg/kg prior to mating, during mating and post mating.

Test Results

Organ	*Effect*	*Rev.*	*OnSet*	*Sex*	*Affected in Exposed - Controls*

NEF

This study revealed no evidence of reproductive toxicity in animals exposed to pre-mating, during mating, and post mating.

NOEL

NOEL for P generation = 1000 mg/kg; NOEL for F1 generation = 1000 mg/kg; NOEL for F2 generation = N/A.

BEHAV

Transient effects on food consumption at 1000 mg/kg.

General Comments : This screening study indicates a low order of concern for reproductive effects in rats. Other diolefins (isoprene) also showed a low order of reproductive toxicity in rats. The following reference is also cited: Melnick, R. L. et al. (1990) Env. Hlth. Persp. 86, 93-98.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 92 MRL 90, (1992)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **TERATOGENICITY**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**
Study type : **LAB**

Test Subject

Organism	*Medium*	*Specification*	*Route*	*Lifestage*	*Sex*	*Number exposed*	*Number controls*
RAT			**ORL**				

Species/strain/system : Sprague-Dawley rats

Test Method and Conditions

Test method description : OECD Protocol on Combination Repeated Dose and Reproductive/Developmental Toxicity Screening; GLP: yes

Exposure

Dose / Concentration : **30-1000 mg/kg**
Exposure comments : Rats were given an oral dose of 30, 100 and 1000 mg/kg prior to mating, during mating and post mating.

Test Results

Organ	*Effect*	*Rev.*	*OnSet*	*Sex*	*Affected in Exposed - Controls*
	NEF				

This study revealed minimal or no treatment related effects.

NOEL

NOEL for maternal animals = 100 mg/kg; NOEL for offsprings = 1000 mg/kg.

BEHAV

Transient decrease in food consumption at 1000 mg/kg.

General Comments : A related isomer (isoprene) demonstrated a low order of developmental toxicity in rats by the inhalation and oral routes of administration. NOAEL for developmental toxicity of 7000 ppm by the inhalation route. This suggests that 1,3-PD is likely to also show a low order of developmental toxicity in rats if studied in a formal inhalation study. The following references are also cited: Tsutsumi, S. et al. (1969) Proc. Congenital Anomalies Res. Assoc., Ann. Report No. 9, 27; Mast, T. J. et al. (1990) Toxicoligist 10, #165.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 92 MRL 90, (1992)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point	:	**AQUATIC ACUTE TOXICITY**
Chemical Name	:	**1,3-Pentadiene**
CAS Number	:	**504-60-9**
Species/strain/system	:	Fathead minnow (Pimephales promelas)
Exposure Period	:	**24-96 h**
Dose / Concentration	:	**6.25-50 mg/L**

Test Method and Conditions

Test method description	:	OECD 203. 1/2 STAT; GLP: yes
Temperature	:	**21.5 C**

Test Results

Organism	*Medium*	*Spec.*	*Route*	*Lifestage*	*Sex*	*Effect*	*Effect Comments*
FISH	**AQ**	**FRESH**		**24wk**		**LC50**	LC50 for 24 hours = 149.4 mg/L; LC50 for 48 hours = 139.9 mg/L; LC50 for 72 hours = 139.9 mg/L; LC50 for 96 hours = 139.9 mg/L.

General Comments : Results are based on measured values. The following reference is also cited: Hamilton, M. A. et al. (1977) Env. Science Tech. 11, 714-719.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 92 MRL 56, (1992)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **AQUATIC TOXICITY**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**

Test Subject

Organism	*Medium*	*Specification*	*Route*	*Lifestage*	*Sex*	*Number exposed*	*Number controls*
ALGAE	**AQ**	**FRESH**		**6d**			

Species/strain/system : Algae (Selenastrum capricornutum)

Test Method and Conditions

Test method description : OECD 201; GLP: yes
Temperature : **24.8 C**

Exposure

Exposure Period : **24-96 h**
Dose / Concentration : **29.6-326 mg/L**

Test Results

Organ	*Effect*	*Rev.*	*OnSet*	*Sex*	*Affected in Exposed - Controls*
	EC50				

EC50 GR for 24 hours = 179.0 mg/L; EC50 GR for 48 hours > 326.0 mg/L; EC50 GR for 72 hours = 293.9 mg/L; EC50 GR for 96 hours = 174.6 mg/L. EC50 GI for 24 hours > 326.0 mg/L; EC50 GI for 48 hours = 263.8 mg/L; EC50 GI for 72 hours = 210.7 mg/L; EC50 GI for 96 hours = 245.8 mg/L.

Maximum concentration at which no effect was observed within the period of the test: 40.6 mg/L. Minimum concentration at which effect was observed within the period of the test: 80.3 mg/L.

General Comments : EC50 GR = Growth Rate. EC50 GI = Growth Inhibition. Results are based on measured values. The following references are also cited: Finney, D. J. (1971) Probit analysis, Third Edition. London, Cambridge, University Press; SAS User's Guide (1985) Statistics, Version 5.18, SAS Institute Inc., Cary, N. C.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 92 MRL 55, (1992)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point : **AQUATIC TOXICITY**
Chemical Name : **1,3-Pentadiene**
CAS Number : **504-60-9**

Test Subject

Organism	*Medium*	*Specification*	*Route*	*Lifestage*	*Sex*	*Number exposed*	*Number controls*
CRUS	**AQ**	**FRESH**		**<24h**			

Species/strain/system : Water flea (Daphnia magna)

Test Method and Conditions

Test method description : OECD 202. 1/2 STAT; GLP: yes
Temperature : **21.5 C**

Exposure

Exposure Period : **24-48 h**
Dose / Concentration : **13.4-274 mg/L**

Test Results

Organ	*Effect*	*Rev.*	*OnSet*	*Sex*	*Affected in Exposed - Controls*
	EC50				

EC50 for 24 hours = 274.0 mg/L; EC50 for 48 hours = 221.5 mg/L.

General Comments : Results are based on measured values. The following references are also cited: Finney, D. J. (1971) Probit analysis, Third Edition. London, Cambridge, University Press; SAS User's Guide (1985) Statistics, Version 5.18, SAS Institute Inc. , Cary, N. C.

References

Primary Reference : **EXBST***
Exxon Biochemical Sciences, Inc., 92 MRL 53, (1992)

Secondary Reference : **!SIDSP***
OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Study

End Point	:	**TERRESTRIAL TOXICITY**
Chemical Name	:	**1,3-Pentadiene**
CAS Number	:	**504-60-9**
General Comments	:	No testing is planned due to low releases into the environment (toxicity to soil dwelling organisms, plants and birds).

References

Secondary Reference : **!SIDSP***

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High Production Volume Chemicals Programme, (1994)

Substance

Chemical Name : **1,3-PENTADIENE**
Reported Name : **1,3-Pentadiene**
CAS Number : **504-60-9**

Area	Type	Subject	Spec.	Description	Level / Summary Information :
GBR	REG	TRNSP	MARIN	RQR	CATEGORY C SUBSTANCE: DISCHARGE INTO THE SEA IS PROHIBITED; DISCHARGE OF TANK WASHINGS AND RESIDUAL MIXTURES IS SUBJECT TO RESTRICTIONS .
		AQ	MARIN	RSTR	
		AQ	EMI	RSTR	

Title : THE MERCHANT SHIPPING (CONTROL OF POLLUTION B Y NOXIOUS LIQUID SUBSTANCES IN BULK) REGULATI ONS 1987, SCHEDULE 1

Reference : **GBRSI*, 551, 15, 1987** ***Effective Date :*** 06APR1987
Statutory Instruments
Last Amendment : **GBRSI*, 2604, 2, 1990** ***Entry / Update :*** 1992
Statutory Instruments

Substance

Chemical Name : **1,3-PENTADIENE**
Reported Name : **1,3-PENTADIENE**
CAS Number : **504-60-9**

Area	Type	Subject	Spec.	Description	Level / Summary Information :
RUS	REG	AIR	AMBI	MAC	0.5MG/M3 1X/D

Title :

Reference : ***Effective Date :*** NOV1989

Last Amendment : **PDKAV*, 5158-89, 1989** ***Entry / Update :*** JUL1990
PREDELNO DOPUSTIMYE KONTSENTRATSII (PDK) ZAGRYAZNYAYUSHCHIKH VESHCHESTV V ATMOSFERNOM VOZDUKHE NASELENNYKH MEST (MAXIMUM ALLOWABLE CONCENTRATIONS (MAC) OF CONTAMINANTS IN THEAMBIENT AIR OF RESIDENTIAL AREAS)

Substance

Chemical Name : **1,3-PENTADIENE**
Reported Name : **PIPERYLENE**
CAS Number : **504-60-9**

Area	Type	Subject	Spec.	Description	Level / Summary Information :
RUS	REG	AIR	OCC	MAC CLASS	CLV: 40.0MG/M3 (VAPOUR) HAZARD CLASS: IV

Title :

Reference : ***Effective Date :*** 01JAN1989

Last Amendment : **GOSTS*, 12.1.005, 1988** ***Entry / Update :*** MAY1990
GOSUDARSTVENNYI STANDART SSSR (STATE STANDARD OF USSR)

Substance

Chemical Name : **1,3-PENTADIENE**
Reported Name : **1,3-PENTADIENE**
CAS Number : **504-60-9**

Area	Type	Subject	Spec.	Description	Level / Summary Information :
RUS	REG	AIR	AMBI	PSL	0.05MG/M3 1X/D

Title :

Reference : ***Effective Date :*** DEC1983

Last Amendment : **OBUAV*, 2947-83, 1983** ***Entry / Update :*** SEP1985

Orientivovochnye bezopasnye urovni vozdeystvya (OBUV) zagryaznyayushchikh veschchestv v atmosfernom vozdukhe naselennykh mest
(Tentative Safe Exposure Limits (TSEL) of contaminants in AmbientAir of Residential Areas)

Substance

Chemical Name : **1,3-PENTADIENE**
Reported Name : **PENTADIENE,1,3-**
CAS Number : **504-60-9**

Area	Type	Subject	Spec.	Description	Level / Summary Information :
USA	REG	CLASS	INDST	RQR	100 (45.4); Summary - RELEASES OF THIS HAZARD OUS SUBSTANCE, IN QUANTITIES EQUAL TO OR GREA TER THAN ITS REPORTABLE QUANTITY (RQ), REPORT ED AS óLBS (KG)|, ARE SUBJECT TO REPORTING TO THE NATIONAL RESPONSE CENTER UNDER THE COMPR EHENSIVE ENVIRONMENTAL RESPONSE, COMPENSATION , AND LIABILITY ACT. (#)- RQ IS SUBJECT TO CH ANGE
		AIR	EMI	RQR	
		AQ	EMI	RQR	

Title : CERCLA: LIST OF HAZARDOUS SUBSTANCES AND REPO RTABLE QUANTITIES

Reference : **CFRUS*, 40, 302, 4, 1990** ***Effective Date :*** 1990
Code of Federal Regulations

Last Amendment : **CFRUS*, 40, 302, 4, 1990** ***Entry / Update :*** SEP1991
Code of Federal Regulations

Substance

Chemical Name : **1,3-PENTADIENE**
Reported Name : **1-METHYLBUTADIENE**
CAS Number : **504-60-9**

Area	Type	Subject	Spec.	Description	Level / Summary Information :
USA	REG	WASTE STORE TRNSP	INDST - REMOV	CLASS RQR RQR	IGNITABLE; Summary - THIS CHEMICAL, IF DISCAR DED, MUST BE TREATED AS AN ACUTE HAZARDOUS WA STE. ACUTE HAZARDOUS WASTES REGULATIONS ARE M ORE RESTRICTIVE FOR EXCLUSION. ANY RESIDUE OF THIS CHEMICAL LABELED AS ACUTELY HAZARDOUS A ND REMAINING IN A CONTAINER, OR AN INNER LINE R R EMOVED FROM A CONTAINER, IS CONSIDERED A HAZARDOUS WASTE IF DISCARDED UNLESS TRIPLE RI NSING OR OTHER CLEANING MEASURES ARE TAKEN (4 0 CFR 261.33E). ***Title :*** RCRA-RESOURCE AND CONSERVATION RECOVERY ACT: DISCARDED COMMERCIAL CHEMICAL PRODUCTS, OFF-S PECIFICATION SPECIES, CONTAINER RESIDUES, AND SPILL RESIDUES THEREOF. ***Reference :*** **FEREAC, 45, 78541, 1980** ***Effective Date :*** 1980 **Federal Register** ***Last Amendment :*** **CFRUS*, 40, 261, 33, 1990** ***Entry / Update :*** JAN1992 **Code of Federal Regulations**

Substance

[redacted]

Chemical Name : **1,3-PENTADIENE**
Reported Name : **1,3-PENTADIENE**
CAS Number : **504-60-9**

Area	Type	Subject	Spec.	Description	Level / Summary Information :
USA	REG	WASTE STORE TRNSP	INDST - REMOV	CLASS RQR RQR	IGNITABLE; Summary - THIS CHEMICAL, IF DISCAR DED, MUST BE TREATED AS AN ACUTE HAZARDOUS WA STE. ACUTE HAZARDOUS WASTES REGULATIONS ARE M ORE RESTRICTIVE FOR EXCLUSION. ANY RESIDUE OF THIS CHEMICAL LABELED AS ACUTELY HAZARDOUS A ND REMAINING IN A CONTAINER, OR AN INNER LINE R R EMOVED FROM A CONTAINER, IS CONSIDERED A HAZARDOUS WASTE IF DISCARDED UNLESS TRIPLE RI NSING OR OTHER CLEANING MEASURES ARE TAKEN (4 0 CFR 261.33E). ***Title :*** RCRA-RESOURCE AND CONSERVATION RECOVERY ACT: DISCARDED COMMERCIAL CHEMICAL PRODUCTS, OFF-S PECIFICATION SPECIES, CONTAINER RESIDUES, AND SPILL RESIDUES THEREOF. ***Reference :*** **FEREAC, 45, 78541, 1980** ***Effective Date :*** 1980 **Federal Register** ***Last Amendment :*** **CFRUS*, 40, 261, 33, 1990** ***Entry / Update :*** JAN1992 **Code of Federal Regulations**

Substance

[redacted]

Chemical Name :
Reported Name : **1,3-Pentadiene**
CAS Number : **504-60-9**

Area	Type	Subject	Spec.	Description	Level / Summary Information :
IMO	REC	AQ AQ	EMI MARIN	RSTR RSTR	Category C substance (substance which is slightly toxic to aquatic life): discharge into the sea of this substance, of ballast water, tank washings or other residues or mixtures containing such a substance shall be prohibited except where specified conditions are satisfied. Technological requirements prescribe equipments and designs that must be present on the tankers as well as port facilities for receiving residues or mixtures containing the regulated substance. Technical assistance for training of scientific and technical personnel shall be promoted where requested by the Parties of the Convention. ***Title :*** International Convention for the Prevention of Pollution from Ships, 1973, as modified by the Protocol of 1978 relating thereto (MARPOL 73/78). ***Reference :*** ***Effective Date :*** ***Last Amendment :*** **IMODC*,** ***Entry / Update :*** SEP1994