OECD SIDS 2-BUTENE

**FOREWORD** 

**INTRODUCTION** 

2-BUTENE CAS N°: 107-07-7

## Substance

End Point : IDENTIFIERS, PHYSICAL AND CHEMICAL PROPERTIES

Chemical Name : 2-Butene
Common Name : 2-Butene
CAS Number : 107-01-7
RTECS Number : EM2932000

## Synonyms

.beta.-Butene .beta.-Butylene

**Pseudobutylene** 

## **Properties & Definitions**

Molecular Formula : C4H8
Molecular Weight : 56.1
State : Gas

Octanol/Water Partition :

Coefficient Impurities log Pow = 1.85

: In Dow Europe product: n-butane 1.11 vol%; 1-butene 0.935 vol%;

isobutylene +/-200 volppm; ethylacetylene <20 volppm; 1,3-butadiene 240 volppm. In shell product: n-butane 41.3%;

isobutylene 0.4%: C5 0.4%.

Definitions : Composed of two structural formes: trans-2-butene and cis-2-butene

100% 2-butene = 70% cis and 30% trans.

#### Overall Evaluation

#### SIDS INITIAL ASSESSMENT

This chemical is presently of low priority.

#### SUMMARY OF REASONS SUPPORTING THE RECOMMENDATION

2-Butene is manufactured in a closed system and used in the production of gasolines, butadiene and other chemicals. Based upon the available information, the initial assessment gave indications for concern at peak concentration for humans and no indications for concern for the aquatic environment.

However, the assessment is considered to be limited by:

- the available exposure data concern only one site in the Netherlands.
- no exposure data for 2-butene per se were available; but only as a part of total C4 chemicals.

# Production-Trade

Chemical Name : 2-Butene
CAS Number : 107-01-7
Geographic Area : EUR
Area Specifications : W

## Production

<u>Quantity</u> <u>Year</u>

20000 T - P/Y

General Comments : No information for other production site.

## References

!SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

Production Volume Chemicals Programme, 4, (1993)

#DOWFU\*

Dow Europe, Unpublished Report or Communications, (1992)

Uses 3

## Uses

Chemical Name : 2-Butene
CAS Number : 107-01-7
Geographic Area : EUR
Area Specifications : W

## Use

<u>Quantity</u> <u>Year</u> <u>Comments</u>

2000-20000 T 1992 Used in the production of gasolines, butadiene and

other chemicals.

# References

Secondary References : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

End Point : Pathway into the Environment and Environmental Fate.

Chemical Name : 2-Butene CAS Number : 107-01-7

## Test Method and Conditions

Test method description

Fugacity model, Mackay level 1

# **Quantity Transported**

<u>Medium</u>	to Medium	<u>Quantity</u>	<u>Time</u>	<u>Year</u>	<u>to Year</u>
(O-1l-tl)	to AIR	99 %			
(Calculated)					
(Calculated)	to AQ	<0.1 %			
	to SOIL	<0.1 %			
(Calculated)					
(Calculated)	to SED	<0.1 %			
	to FISH	>0.1 %			
(Calculated)					

>0.1 %

More than 0.1% in suspended matters (calculated value). From these calculations it can be concluded that almost all 2-butene will partition into the atmosphere.

General Comments : Based on emissions from cracking installations for the production of other

chemicals e.g. ethene, butadiene and propene, an emission factor of 0.02% and 0.2% was estimated for production and processing respectively.

## References

Primary Reference : CMSHAF

Mackay, M., et al. Chemosphere. Chemistry, Biology and Toxicology as related

to Environmental Problems, 23(6), 695-717, (1992)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

Production Volume Chemicals Programme, (1993)

# Study

End Point : Pathway into the Environment and Environmental Fate.

Chemical Name : 2-Butene CAS Number : 107-01-7

#### **Test Method and Conditions**

Test method description

Screening Assessment Model System (SAMS) Plume model.

IRPTC Data Profile

# **Quantity Transported**

<u>Medium</u> <u>to Medium</u> <u>Quantity</u> <u>Time</u> <u>Year</u> <u>to Year</u>

to AIR

Concentration: 4.84E-11mg/m3 (330m from the emission point, height 50m) calculations based on plume model

#### References

Primary Reference : OECDM\*

OECD Screening Assessment Model System (SAMS), (1992)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

Production Volume Chemicals Programme, 6, (1993)

## Study

End Point : Pathway into the Environment and Environmental Fate.

Chemical Name : 2-Butene CAS Number : 107-01-7

## Pathway and Transport

Pathway : AIR

Pathway description : Evaporation

# **Quantity Transported**

<u>Medium</u> <u>to Medium</u> <u>Quantity</u> <u>Time</u> <u>Year</u> <u>to Year</u>

to AIR 4.2 %

Evaporation from gasoline fuel tank: 4.2 vol% of total evaporated hydrocarbons.

to AIR 0.2-0.3 %

Evaporation from carburator: 0.2-0.3 vol% of total evaporated hydrocarbons.

to AIR 0.6 %

In exhaust of diesel engine: 0.6% of emitted hydrocarbons.

#### References

Primary Reference : HBEDC\*

Verchueren, K. Handbook of Environmental Data on Organic Chemicals,

(1987)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

End Point : HUMAN INTAKE AND EXPOSURE

Chemical Name : 2-Butene CAS Number : 107-01-7

# Test Subject

Organism Medium Specification Route Lifestage Sex

HUMAN IHL

Species/strain/system : Average exposure 8hours. Exposition due to leaking in craking

installations and during transport.

## **Test Results**

<u>Intake</u> <u>Spec.</u> <u>Date</u>

#### 11.5 mg/m3

EHE max (maximum estimated human exposure) = 5ppm or 11.5 mg/m3 equivalent to the peak concentration at working place.

#### <0.23 mg/m3

TWA (time-weighted average) at working place or EHE mean <0.1ppm, (calculated).

General Comments : EHE based on measurement of C4 chemicals.

#### References

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

End Point : PHOTODEGRADATION

Chemical Name : 2-Butene
CAS Number : 107-01-7
Study type : LAB
Medium : AIR

#### **Test Method and Conditions**

Test method : Unknown

description

Temperature : 27 C

#### **Test Results**

Quantity <u>Time</u> <u>Comments on result</u>

**50 %** LOSS **0.3 h** T/2 with NO

50 % LOSS 10-11 mi T/2 with NO2. The reported time is 0.17 hours.

General Comments: Levels of 2-butene in air will be low due to the rapid photodegradation.

#### References

Primary Reference : ESTHAG

Dilling, W. L., et al. Environmental Science and Technology, 10(4), 351-

356, (1976)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

Production Volume Chemicals Programme, 7, (1993)

## Study

End Point : PHOTODEGRADATION

Chemical Name : 2-Butene
CAS Number : 107-01-7
Study type : LAB
Medium : AIR

## Test Substance

Description of the test : cis-2-Butene and trans-2-butene

substance

#### Test Method and Conditions

Test method : Unknown

description

Temperature : 25 C

# **Test Results**

Quantity <u>Time</u> <u>Comments on result</u>

Reaction with hydroxyl radicals both measured at 25C. Reaction constants are: cis-butene: k = 5.6E-5/s, trans-2-butene: k = 6.4E-5/s. At

lower temperatures reaction constants will be higher.

References

Primary Reference : CHREAY

Atkinson, R. Chemical Reviews, 85, 69-201, (1980)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

Hydrolysis

# Study

End Point : HYDROLYSIS
Chemical Name : 2-Butene
CAS Number : 107-01-7
Study type : LAB
Medium : AQ
Specifications : FRESH

Test Substance

Description of the test

substance

cis-2-Butene and trans-2-butene

Test Method and Conditions

Test method description

Unknown

Exposure

Dose / Concentration : The release of both isomers from an aqueous solution was tested at 5

concentrations.

**Test Results** 

Quantity <u>Time</u> Comments on result

**700 mg/l 3 h** After maximum 3 hours, the observed levels showed a decrease from

700mg/l to <1mg/l (detection limit). DT5O is 5-25 minutes, depending on

the concentration tested (at ambient temperature).

References

Primary Reference : #DOWEU\*

Dow Europe, Unpublished Report or Communications, (1992)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

End Point : MAMMALIAN ACUTE TOXICITY

Chemical Name : 2-Butene CAS Number : 107-01-7

**Test Results** 

Organism Medium Spec. Route Lifestage Sex Effect Effect Comments

MOUSE IHL ADULT LC50 Mouse inhalation LC50 was estimated

as 977mg/m3.

References

Primary Reference : RTECS\*

Anonymous. Registry of Toxic Effects of Chemical Substances, (1986)

Secondary Reference : SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

Production Volume Chemicals Programme, 7, (1993)

Study

End Point : MAMMALIAN ACUTE TOXICITY

Chemical Name : 2-Butene CAS Number : 107-01-7

Exposure Period : 4 h

**Test Method and Conditions** 

Test method description

OECD No. 403, GLP: yes.

**Test Results** 

Organism Medium Spec. Route Lifestage Sex Effect Effect Comments

RAT IHL ADULT LC50 Rat inhalation LC50 was estimated as

>23.1g/m3.

References

Primary Reference : #RHVTDT

Arts, J. H. E. TNO Central Institute for Nutrition and Food Research Report-Netherlands Organization for Applied Scientific Research, Division for Nutrition

and Food Research, (1992)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

End Point : MAMMALIAN TOXICITY

Chemical Name : 2-Butene
CAS Number : 107-01-7
Study type : LAB

## Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls

RAT IHL ADULT M

Species/strain/system : Wistar albino (Hsd/Cpd: WU)

#### Test Substance

Description of the test :

substance

2-Butene (cis-2-butene 42.4%, trans-2-butene 55.3%)

#### Test Method and Conditions

Test method : OECD Combined Repeated Dose Reproductive/Developmental Toxicity

description Screening Test. GLP: yes.

**Exposure** 

Exposure Period : 39-46 d
Frequency : 6 h/d
7 d/wk

Dose / Concentration : 5.7-11.5 g/m3

Exposure comments : Doses were 0, 5.7, and 11.5g/m3.

#### **Test Results**

Affected in

Organ Effect Rev. OnSet Sex Exposed - Controls

NEF

No Adverse Effect Level (NOAEL) was at the dose level of 5.7g/m3.

**BW DECR F** Body weight decrease was observed at the dose level of 11.5g/m3.

BEHAV F

Food consumption was decreased at the dose level of 11.5g/m3.

BLOOD BIOCH M

At the dose level of 11.5g/m3 calcium levels of blood plasma were decreased.

General Comments : Estimated dose of low concern (EDLC) was calculated as = 11.4mg/m3 using

an uncertainty factor of 500.

# References

Primary Reference : #RHVTDT

Waalkens Berendsen, D. H. and Arts, J. H. E. TNO Central Institute for Nutrition and Food Research Report-Netherlands Organization for Applied Scientific Research, Division for Nutrition and Food Research, (1992)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

Mutagenicity 1

# Study

End Point : MUTAGENICITY

Chemical Name : 2-Butene
CAS Number : 107-01-7
Study type : LAB

## Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls

BACT VTR

Species/strain/system : Salmonella Typhimurium TA98, TA100,TA1535,TA1537

#### Test Method and Conditions

Test method description

OECD No. 471; Safefarm definitive protocol Tx 3569(amended). GLP: yes.

**Exposure** 

Exposure Period : 10-80 %

Exposure comments : Doses of 10, 20, 40, 60, or 80% tested with and without metabolic activation.

Positive control with and without S9 mix were included. Negative control:

clean, dry air. 2 replicates.

**Test Results** 

Affected in

Organ Effect Rev. OnSet Sex Exposed - Controls

NEF

Negative results with and without metabolic activation.

CHNG

Minimum concentration at which toxicity to bacteria was observed is 60%.

#### References

Primary Reference : #URSPH\*

Thompson, P. W. Unpublished Report - Safepharm, 44/182 D.D. 6-04, (1992)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

End Point : MUTAGENICITY

Chemical Name : 2-Butene
CAS Number : 107-01-7
Study type : LAB

## Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls

RAT VTR

Species/strain/system : Rat lymphocytes

## Test Substance

Description of the test

substance

cis-2-Butene 42.2% and trans-2-butene 55.3%.

#### Test Method and Conditions

Test method description

OECD No: 473; Safefarm definitive protocol Tx3570 (amended). GLP: yes.

Exposure

Exposure Type : SHORT

Dose / Concentration : 40-60 %

Exposure comments : Concentrations: 40, 50, or 60% of cis-2-butene and trans-2-butene mixed with

dry air. Positive control: -S9 mix: (EMS). Positive control: +S9 mix:

cyclophosphamide (CP), vinylchloride 50%. Negative control: clean dry air.

Harvest time 20, 30 hours.

## **Test Results**

Affected in

Organ Effect Rev. OnSet Sex Exposed - Controls

CELL

Lowest concentration producing cell toxicity: > 60% with and without metabolic activation.

NEF

Genotoxic effect was absent with and without metabolic activation under the test conditions.

#### References

Primary Reference : #URSPH\*

Unpublished Report - Safepharm, (1992)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

End Point : REPRODUCTION

Chemical Name : 2-Butene
CAS Number : 107-01-7
Study type : LAB

## Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls

RAT IHL M

Species/strain/system : Wistar albino rats (Had/Cpd: WU)

## Test Method and Conditions

Test method : OECD Combined Repeated Dose and Reproductive/Developmental Toxicity

description Screening Test. GLP: yes.

Exposure

Frequency : 6 h/d

7 d/wk

Dose / Concentration : 5.7-11.5 g/m3

**Test Results** 

Affected in

Organ Effect Rev. OnSet Sex Exposed - Controls

NEF

No Adverse Effect Level for the parental generation was reported as = 5.7g/m3.

NEF

No Adverse Effect Level for F1 generation was reported as 11.5g/m3. Effective dose of low concern (repro.) was calculated as = 23mg/m3.

NEF

No effects on the number of pups born, sex, ratio and viability index.

## References

Primary Reference : #RHVTDT

Waalkens - Berendsen D. H. and Arts, J. H. E. TNO Central Institute for Nutrition and Food Research Report-Netherlands Organization for Applied Scientific Research, Division for Nutrition and Food Research, (1992)

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

End Point : AQUATIC ACUTE TOXICITY

Chemical Name : 2-Butene CAS Number : 107-01-7

Species/strain/system : Fathead minnow (Pimephales promelas)

Exposure Period : 96 h

## Test Method and Conditions

Test method description

Estimation of aquatic effects data for 2-butene using Quantitative Structure-Activity Relationships (QSAR's) using the equation log LC50 = -0.85 log kow -

1.41. Value of  $\log kow = 1.85$ .

## **Test Results**

Organism Medium Spec. Route Lifestage Sex Effect Effect Comments

FISH AQ FRESH LC50 LC50 = 58mg/l.

General Comments : QSAR's can be used to estimate the toxicity of a compound. 2-Butene can be

classified as an inert chemical which acts by a narcosis-type or baseline

toxicity.

## References

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

End Point : AQUATIC TOXICITY

Chemical Name : 2-Butene CAS Number : 107-01-7

Test Subject

Organism Medium Specification Route Lifestage Sex Number exposed Number controls

CRUS AQ FRESH

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

**Test Method and Conditions** 

Test method description

Estimation of aquatic effects data for 2-butene using Quantitative Structure-Activity Relationships (QSAR's) using the equation log EC50 = -0.95 log

kow -1.19, and log kow = 1.85.

Exposure

Exposure Type : ACUTE Exposure Period : 48 h

**Test Results** 

Affected in

Organ Effect Rev. OnSet Sex Exposed - Controls

EC50

EC50 = 63 mg/l.

General Comments : QSAR's can be used to estimate the toxicity of a compound. 2-Butene can be

classified as an inert chemical which acts by a narcosis-type or baseline

toxicity.

References

Secondary Reference : !SIDSP\*

OECD/SIDS. Screening Information Data Set (SIDS) of OECD High

Substance

Chemical Name :

Reported Name : 2-butene CAS Number : 107-01-7

Area Type Subject Spec. Description Level / Summary Information:

DEU REG CLASS - CLASS

LABEL RQR PACK RQR CLASSIFICATION AND LABELLING IN GERMANY IS GENERALLY THE SAME AS FOR THE EEC (SEE OJEC\*\* L180, 1991). HOWEVER, SLIGHT MODIFICATIONS MAY BE

INTRODUCED FOR SOME SUBSTANCES IN THE GERMAN LEGISLATION.

 Title:
 ORDINANCE ON HAZARDOUS SUBSTANCES. (GEFAHRSTOFFVERORDNUNG)

 Reference:
 :
 BGZBAD, I, 1931, 1991
 Effective Date:
 15JUN1991

Bundesgesetzblatt. Federal Law Gazette

<u>Last Amendment</u>: <u>Entry / Update</u>: APR1992

Substance

Chemical Name :

Reported Name : 2-butene CAS Number : 107-01-7

Area Type Subject Spec. Description Level / Summary Information:

RUS REG AIR AMBI MAC 3.0MG/M3 1X/D, 3.0MG/M3 AV/D (APPLIES TO BUTENE ISOMERS MIXTURE)

Title :

Reference : Effective Date : AUG1984

<u>Last Amendment :</u> PDKAV\*, 3086-84, 1984 <u>Entry / Update :</u> SEP1985

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 :

Reported Name : 2-butene CAS Number : 107-01-7

Area Type Subject Spec. Description Level / Summary Information:

RUS REG AQ SURF MAC 0.2 MG/L (APPLIES TO ALL BUTENE ISOMERS) HAZARD CLASS: III

CLASS <u>Title</u>:

<u>Reference</u>: 1JAN1989

<u>Last Amendment :</u> SPNPV\*, 4630-88, 1988 <u>Entry / Update :</u> JUL1990

SANITARNYE PRAVILA I NORMY OKHRANY POVERKHNOSTNYKH

VOD OT ZAGRIAZNENIA

(HEALTH REGULATION AND STANDARDS OF SURFACE WATER

PROTECTION FROM CONTAMINATION)

#### Substance

Chemical Name :

Reported Name : 2-butene CAS Number : 107-01-7

Area Type Subject Spec. Description Level / Summary Information:

EEC REG FOOD

PACK ADDIT PRMT

THIS SUBSTANCE MAY BE USED FOR THE MANUFACTURE OF PLASTICS MATERIALS AND ARTICLES INTENDED TO COME INTO CONTACT WITH FOODSTUFFS. THESE PLASTICS MATERIALS AND ARTICLES SHALL NOT TRANSFER THEIR CONSTITUENTS IN QUANTITIES EXCEEDING 10 MG/DM2 OF SURFACE AREA OF MATERIAL OR ARTICLE (OVERALL MIGRATION LIMIT) OR 60 MG/KG OF FOODSTUFF, FOR CERTAIN CONTAINERS OR SEALING DEVICES. THE BASIC RULES FOR TESTING MIGRATION OF THE CONSTITUENTS OF PLASTICS MATERIALS AND ARTICLES ARE LAID DOWN IN DIRECTIVE 82/711/EEC (OJEC L297,26,1982) AND THE LIST OF SIMULANTS TO BE USED IN THE MIGRATION TESTS IS GIVEN IN DIRECTIVE 85/572/EEC (OJEC L372, 14, 1985).

<u>Title</u>: COMMISSION DIRECTIVE OF 23 FEBRUARY 1990 RELATING TO PLASTICS MATERIALS AND ARTICLES INTENDED TO COME INTO CONTACT WITH

FOODSTUFFS (90/128/EEC).

<u>Reference</u>: OJEC\*\*, L75, 19, 1990 <u>Effective Date</u>: 31DEC1990

Official Journal of the European Communities

Last Amendment: Entry / Update: 1991

#### Substance

Chemical Name :

Reported Name : 2-butene CAS Number : 107-01-7

Area Type Subject Spec. Description Level / Summary Information:

EEC REG CLASS - CLASS

LABEL RQR PACK RQR CLASS: F - HIGHLY FLAMMABLE; EXTREMELY FLAMMABLE LIQUEFIED GAS (R 13). LABEL: F - HIGHLY FLAMMABLE; EXTREMELY FLAMMABLE LIQUEFIED GAS (R 13); KEEP CONTAINER IN A WELL-VENTILATED PLACE (S 9); KEEP AWAY FROM SOURCES OF IGNITION - NO SMOKING (S 16); TAKE PRECAUTIONARY MEASURES AGAINST STATIC DISCHARGES (S 33). IT SHOULD BE STATED ON THE LABEL WHETHER IT IS A SPECIFIC ISOMER OR A MIXTURE OF ISOMERS.

Title: COUNCIL DIRECTIVE 67/548/EEC OF 27 JUNE 1967 ON THE APROXIMATION OF THE LAWS, REGULATIONS AND ADMINISTRATIVE PROVISIONS RELATING TO THE CLASSIFICATION, PACKAGING AND LABELLING OF DANGEROUS SUBSTANCES

<u>Reference</u> : OJEC\*\*, 196, 1, 1967 <u>Effective Date</u> : 1JUL1992

Official Journal of the European Communities

<u>Last Amendment :</u> OJEC\*\*, L 180, 79, 1991 <u>Entry / Update :</u> APR1992

Official Journal of the European Communities