

Behavioral – General anesthetic**4.0 STANDARDS AND REGULATIONS▲**

1. OEL IN ARGENTINA, BULGARIA, COLOMBIA, JORDAN, KOREA check ACGIH TLV;
2. OEL IN NEW ZEALAND, SINGAPORE, VIETNAM check ACGIH TLV
3. OEL-GERMANY: MAK 2400 mg/m³ (1000 mL/m³), 2005
4. OEL-SWITZERLAND: MAK-W 800 ppm (1900 mg/m³), JAN1999

5.0 NIOSH DOCUMENTS▲

1. National Occupational Exposure Survey 1983: Hazard Code 81851; Number of Industries 377; Total Number of Facilities 110810; Number of Occupations 233; Total Number of Employees 1795168; Total Number of Female Employees 556159
2. National Occupational Hazard Survey 1974: Hazard Code 81851; Number of Industries 360; Total Number of Facilities 118992; Number of Occupations 199; Total Number of Employees 1193478

6.0 REVIEWS▲

1. ACGIH TLV-TWA 1000 ppm
2. TOXICOLOGY REVIEW

7.0 STATUS IN U.S.▲

1. EPA TSCA Section 8(b) CHEMICAL INVENTORY
2. EPA TSCA Section 8(d) unpublished health/safety studies
3. EPA TSCA TEST SUBMISSION (TSCATS) DATA BASE, JANUARY 2001

資料B-6(HSDB)

ISOBUTANE

HSDB - Hazardous Substances Data Bank

0.0 ADMINISTRATIVE INFORMATION

Hazardous Substances Data Bank Number: 608

Last Revision Date: 20030214

Review Date: Reviewed by SRP on 5/16/1996

Update History:

1. Complete Update on 02/14/2003, 1 field added/edited/deleted.
2. Complete Update on 01/24/2003, 2 fields added/edited/deleted.
3. Field Update on 11/08/2002, 1 field added/edited/deleted.
4. Complete Update on 01/18/2002, 3 fields added/edited/deleted.
5. Complete Update on 08/09/2001, 1 field added/edited/deleted.
6. Complete Update on 05/15/2001, 1 field added/edited/deleted.
7. Complete Update on 02/08/2000, 1 field added/edited/deleted.
8. Complete Update on 02/02/2000, 1 field added/edited/deleted.
9. Complete Update on 11/18/1999, 1 field added/edited/deleted.
10. Complete Update on 09/21/1999, 1 field added/edited/deleted.
11. Complete Update on 07/27/1999, 4 fields added/edited/deleted.
12. Complete Update on 03/19/1999, 1 field added/edited/deleted.
13. Complete Update on 10/17/1997, 1 field added/edited/deleted.
14. Complete Update on 07/08/1997, 2 fields added/edited/deleted.
15. Complete Update on 04/01/1997, 2 fields added/edited/deleted.
16. Complete Update on 08/19/1996, 70 fields added/edited/deleted.
17. Field Update on 01/19/1996, 1 field added/edited/deleted.
18. Complete Update on 05/26/1995, 1 field added/edited/deleted.
19. Complete Update on 12/21/1994, 1 field added/edited/deleted.
20. Complete Update on 08/18/1994, 1 field added/edited/deleted.
21. Complete Update on 03/25/1994, 1 field added/edited/deleted.
22. Complete Update on 02/05/1993, 1 field added/edited/deleted.
23. Field update on 12/14/1992, 1 field added/edited/deleted.
24. Complete Update on 12/08/1992, 1 field added/edited/deleted.
25. Complete Update on 11/26/1992, 1 field added/edited/deleted.
26. Complete Update on 10/10/1990, 1 field added/edited/deleted.
27. Complete Update on 04/16/1990, 1 field added/edited/deleted.
28. Field update on 12/29/1989, 1 field added/edited/deleted.
29. Complete Update on 04/13/1989, 1 field added/edited/deleted.
30. Complete Update on 04/24/1987

1.0 SUBSTANCE IDENTIFICATION

Name of Substance: ISOBUTANE

CAS Registry Number: 75-28-5

Synonyms:

1. 1,1-DIMETHYLETHANE [Peer reviewed]
2. 2-METHYLPROPANE [Peer reviewed]
3. ISO-BUTANE [Peer reviewed]
4. ISOBUTANE (DOT) [Peer reviewed] [U.S. Department of Health, Education & Welfare, Public Health Service. Center for Disease Control, National Institute for Occupational Safety & Health. Registry of Toxic Effects of Chemical Substances. 1977 edition. Washington, D. C.: U.S. Government Printing Office, 1977., p. 755]
5. TRIMETHYLMETHANE [Peer reviewed]

Molecular Formula: C4-H10 [Peer reviewed]

Shipping Name/Number – DOT/UN/NA/IMCO:

1. IMO 2.1 – Isobutane
2. UN 1969 – Isobutane

2.0 MANUFACTURING/USE INFORMATION

Methods of Manufacturing:

1. ISOLATION FROM WET NATURAL GAS AND FROM CRUDE PETROLEUM [Peer reviewed]
2. Recovery from petroleum refinery streams that result from catalytic cracking, catalytic reforming and other refinery operations. [Peer reviewed] [Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991–Present., p. V13 820]
3. Isomerization of n-butane. [Peer reviewed] [Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed. Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA13 237]
4. Recovery from raw natural gas which contains about 0.35 mol % isobutane. [Peer reviewed] [Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991–Present., p. V13 820]

Impurities:

0.1% /BUTANE/ [Peer reviewed] [Fluka; Catalog 14, Chemicals and Biochemicals p.672(1984)]

Formulations/Preparations:

Technical, 99 mol % (pure grad), 99.96 mole % (research grade), and other high-purity grades. [Peer reviewed] [Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 12th ed. New York, NY: Van Nostrand Rheinhold Co., 1993, p. 651]

Manufacturers:

R S A Corporation, 36 Old Sherman Turnpike, Danbury, CT 06812, (203)790-8100 [Peer reviewed] [SRI. 1995 Directory of Chemical Producers-United States of America. Menlo Park, CA: SRI International, 1995, p. 763]

Other Manufacturing Information:

1. The most common separation techniques are based on a vapor-liquid, two-phase system by which the liquid (iso)butane is recovered from the feed gas. [Peer reviewed] [Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991–Present., p. V13 820-1]
2. Colorless gas. [Note: Shipped as a liquefied compressed gas. A liquid below 11 degrees F.]

[Peer reviewed] [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 94-116. Washington, D.C.: U.S. Government Printing Office, June 1994., p. 176]

Major Uses:

1. CHEM INT FOR ALKYLATE GASOLINE; COMPONENT TO CONTROL VOLATILITY OF GASOLINE; CHEM INT FOR PROPYLENE OXIDE, TERT-BUTYL ALCOHOL [Peer reviewed]
2. Blended directly into motor fuel to control fuel's volatility. [Peer reviewed] [Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V13 822]
3. Alkylated with C3-C4 olefins to produce highly branched C7-C8 hydrocarbons that are used to raise octane rating. [Peer reviewed] [Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V13 822]
4. Organic synthesis, refrigerant, motor fuels, aerosol propellant, synthetic rubber, instrument calibration fluid. [Peer reviewed] [Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 12th ed. New York, NY: Van Nostrand Reinhold Co., 1993, p. 651]
5. Reactant in the production of propylene oxide by peroxidation of propylene. [Peer reviewed] [Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V13 822]
6. Used alone or in mixtures as hydrocarbon propellants in aerosols. [Peer reviewed] [Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V13 822]
7. Liquid-phase autooxidation to give tert-butylhydroperoxide. [Peer reviewed] [Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed. Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA13 237]
8. Catalytic dehydrogenation to form isobutene, a precursor for methyl tert-butyl ether. [Peer reviewed] [Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed. Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA13 237]
9. Oxidation to produce methacrylic acid. [Peer reviewed] [Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed. Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA13 237]

Consumption Patterns:

1. APPROX 94% AS A CHEM INT FOR ALKYLATE GASOLINE; APPROX 4% AS COMPONENT TO CONTROL VOLATILITY OF GASOLINE; & APPROX 2% AS A CHEM INT FOR PROPYLENE OXIDE & TERT-BUTYL ALCOHOL (1975) [Peer reviewed]
2. In 1987, about 89% of isobutane consumption in the US was motor fuel alkylate. [Peer reviewed] [Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY. John Wiley and Sons, 1991-Present., p. V13 822]

U.S. Production:

1. (1972) 4.28X10+11 GRAMS [Peer reviewed]
2. (1975) 3.39X10+11 GRAMS [Peer reviewed]
3. (1984) 4.80x10+11 g [Peer reviewed] [USITC. SYN ORG CHEM-U.S. PROD/SALES 1984 p.15]

3.0 CHEMICAL AND PHYSICAL PROPERTIES

Color/Form: COLORLESS GAS [Peer reviewed] [Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 12th ed. New York, NY: Van Nostrand Reinhold Co., 1993, p. 651]

Odor:

1. Gasoline-like or natural gas odor. [Peer reviewed] [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 94-116. Washington, D.C.: U.S. Government Printing Office, June 1994., p. 176]
2. Slight [Peer reviewed] [Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 12th ed. New York, NY: Van Nostrand Rheinhold Co., 1993, p. 651]

Boiling Point: -11.7 deg C [Peer reviewed] [Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 75th ed. Boca Raton, Fl: CRC Press Inc., 1994-1995., p. 3-275]

Melting Point: -138.3 DEG C [Peer reviewed] [Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 75th ed. Boca Raton, Fl: CRC Press Inc., 1994-1995., p. 3-275]

Molecular Weight: 58.12 [Peer reviewed] [Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 75th ed. Boca Raton, Fl: CRC Press Inc., 1994-1995., p. 3-275]

Corrosivity: No corrosive action on metals. [Peer reviewed] [Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 12th ed. New York, NY: Van Nostrand Rheinhold Co., 1993, p. 651]

Critical Temperature and Pressure: Critical temperature = 134.69 deg C; critical pressure = 35.82 atm [Peer reviewed] [Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 81]

Density/Specific Gravity: 0.55092 g/cu cm @ 25 deg C; 0.55711 g/cu cm @ 20 deg C; 0.61415 @ -29.5 deg C [Peer reviewed] [Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 80]

Heat of Combustion: -680.84 kcal/mol @ 25 deg C (liquid); -685.71 kcal/mol @ 25 deg C (gas) [Peer reviewed] [Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 81]

Heat of Vaporization: 4.570 kcal/mol @ 25 deg C [Peer reviewed] [Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 81]

Octanol/Water Partition Coefficient: Log Kow = 2.76 [QC reviewed] [Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society., 1995., p. 10]

Solubilities:

1. SOL IN ALCOHOL, ETHER, CHLOROFORM [Peer reviewed] [Lide, D.R. (ed.). CRC Handbook of Chemistry and Physics. 75th ed. Boca Raton, Fl: CRC Press Inc., 1994-1995., p. 3-275]
2. In water: 48.9 mg/L @ 25 deg C [Peer reviewed] [McAuliffe C; J Phys Chem 70: 1267-75 (1966)]

Spectral Properties:

1. IR: 2285 (Sadler Research Laboratories Prism Collection) [Peer reviewed] [Weast, R.C. and M.J. Astle. CRC Handbook of Data on Organic Compounds. Volumes I and II. Boca Raton, FL: CRC Press Inc. 1985., p. V1 315]
2. MASS: 33 (Atlas of Mass Spectral Data, John Wiley & Sons, New York) [Peer reviewed] [Weast, R.C. and M.J. Astle. CRC Handbook of Data on Organic Compounds. Volumes I and II. Boca Raton, FL: CRC Press Inc. 1985., p. V1 315]
3. Refractive index: 1.3175 @ 25 deg C; 1.3209 @ 20 deg C; 1.3524 @ -24.3 deg C [Peer

reviewed] [Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 80]

Surface Tension: 14.1 dyne/cm @ -10 deg C [Peer reviewed] [Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 81]

Vapor Density: 2.01 (AIR= 1) [Peer reviewed] [Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 12th ed. New York, NY: Van Nostrand Reinhold Co., 1993, p. 651]

Vapor Pressure: 2611 mm Hg (348.1 kPa) @ 25 deg C; 391.02 mm Hg (52.132 kPa) @ -27.57 deg C [Peer reviewed] [Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 80]

Viscosity: 0.238 cP @ -10 deg C [Peer reviewed] [Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 81]

Other Chemical/Physical Properties:

1. Heat capacity at constant pressure = 23.10 cal/K-mol @ 25 deg C [Peer reviewed] [Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 81]
2. Dielectric constant: 1.002564 @ 25 deg C (gas); 1.734 @ 25 deg C (liquid) [Peer reviewed] [Riddick, J.A., W.B. Bunger, Sakano T.K. Techniques of Chemistry 4th ed., Volume II. Organic Solvents. New York, NY: John Wiley and Sons., 1985., p. 81]
3. Stable, does not react with water. [Peer reviewed] [Lewis, R.J., Sr (Ed.). Hawley's Condensed Chemical Dictionary. 12th ed. New York, NY: Van Nostrand Reinhold Co., 1993, p. 651]
4. Thermal conductivity: 0.0140 @ 0 deg C; 0.0185 watt/m-K @ 50 deg C [Peer reviewed] [Kirk-Othmer Encyclopedia of Chemical Technology. 4th ed. Volumes 1: New York, NY: John Wiley and Sons, 1991-Present., p. V13 818]
5. hydroxyl radical rate constant = 2.34×10^{-12} cu-cm/molc sec @ 25 deg C [QC reviewed] [Atkinson R; Journal of Physical And Chemical Reference Data. Monograph No 1 (1989)]

4.0 SAFETY AND HANDLING

EMERGENCY GUIDELINES ▲

DOT Emergency Guidelines:

1. /GUIDE 115: GASES – FLAMMABLE (INCLUDING REFRIGERATED LIQUIDS)/ Fire or Explosion: EXTREMELY FLAMMABLE. Will be easily ignited by heat, sparks or flames. Will form explosive mixtures with air. Vapors from liquefied gas are initially heavier than air and spread along ground. ... Vapors may travel to source of ignition and flash back. Cylinders exposed to fire may vent and release flammable gas through pressure relief devices. Containers may explode when heated. Ruptured cylinders may rocket. [QC reviewed] [U.S. Department of Transportation. 2004 Emergency Response Guidebook. A Guide book for First Responders During the Initial Phase of a Dangerous Goods/Hazardous Materials Incident. Washington, D.C. 2004G-115]
2. /GUIDE 115: GASES – FLAMMABLE (INCLUDING REFRIGERATED LIQUIDS)/ Health: Vapors may cause dizziness or asphyxiation without warning. Some may be irritating if inhaled at high concentrations. Contact with gas or liquefied gas may cause burns, severe injury and/or frostbite. Fire may produce irritating and/or toxic gases. [QC reviewed] [U.S. Department of Transportation. 2004 Emergency Response Guidebook. A Guide book

- for First Responders During the Initial Phase of a Dangerous Goods/Hazardous Materials Incident. Washington, D.C. 2004G-115]
3. /GUIDE 115: GASES – FLAMMABLE (INCLUDING REFRIGERATED LIQUIDS)/ Public Safety: CALL Emergency Response Telephone Number. ... As an immediate precautionary measure, isolate spill or leak area for at least 100 meters (330 feet) in all directions. Keep unauthorized personnel away. Stay upwind. Many gases are heavier than air and will spread along ground and collect in low or confined areas (sewers, basements, tanks). Keep out of low areas. [QC reviewed] [U.S. Department of Transportation. 2004 Emergency Response Guidebook. A Guide book for First Responders During the Initial Phase of a Dangerous Goods/Hazardous Materials Incident. Washington, D.C. 2004G-115]
 4. /GUIDE 115: GASES – FLAMMABLE (INCLUDING REFRIGERATED LIQUIDS)/ Protective Clothing: Wear positive pressure self-contained breathing apparatus (SCBA). Structural firefighters' protective clothing will only provide limited protection. Always wear thermal protective clothing when handling refrigerated/cryogenic liquids. [QC reviewed] [U.S. Department of Transportation. 2004 Emergency Response Guidebook. A Guide book for First Responders During the Initial Phase of a Dangerous Goods/Hazardous Materials Incident. Washington, D.C. 2004G-115]
 5. /GUIDE 115: GASES – FLAMMABLE (INCLUDING REFRIGERATED LIQUIDS)/ Evacuation: Large spill: Consider initial downwind evacuation for at least 800 meters (1/2 mile). Fire: If tank, rail car or tank truck is involved in a fire, ISOLATE for 1600 meters (1 mile) in all directions; also, consider initial evacuation for 1600 meters (1 mile) in all directions. [QC reviewed] [U.S. Department of Transportation. 2004 Emergency Response Guidebook. A Guide book for First Responders During the Initial Phase of a Dangerous Goods/Hazardous Materials Incident. Washington, D.C. 2004G-115]
 6. /GUIDE 115: GASES – FLAMMABLE (INCLUDING REFRIGERATED LIQUIDS)/ Fire: DO NOT EXTINGUISH A LEAKING GAS FIRE UNLESS LEAK CAN BE STOPPED. ... Small fires: Dry chemical or CO2. Large fires: Water spray or fog. Move containers from fire area if you can do it without risk. Fire involving tanks: Fight fire from maximum distance or use unmanned hose holders or monitor nozzles. Cool containers with flooding quantities of water until well after fire is out. Do not direct water at source of leak or safety devices; icing may occur. Withdraw immediately in case of rising sound from venting safety devices or discoloration of tank. ALWAYS stay away from tanks engulfed in fire. For massive fire, use unmanned hose holders or monitor nozzles; if this is impossible, withdraw from area and let fire burn. [QC reviewed] [U.S. Department of Transportation. 2004 Emergency Response Guidebook. A Guide book for First Responders During the Initial Phase of a Dangerous Goods/Hazardous Materials Incident. Washington, D.C. 2004G-115]
 7. /GUIDE 115: GASES – FLAMMABLE (INCLUDING REFRIGERATED LIQUIDS)/ Spill or Leak: ELIMINATE all ignition sources (no smoking, flares, sparks or flames in immediate area). All equipment used when handling the product must be grounded. Do not touch or walk through spilled material. Stop leak if you can do it without risk. If possible, turn leaking containers so that gas escapes rather than liquid. Use water spray to reduce vapors or divert vapor cloud drift. Avoid allowing water runoff to contact spilled material. Do not direct water at spill or source of leak. Prevent spreading of vapors through sewers, ventilation systems and confined areas. Isolate area until gas has dispersed. CAUTION: When in contact with refrigerated/cryogenic liquids, many materials become brittle and are likely to break without warning. [QC reviewed] [U.S. Department of Transportation. 2004 Emergency Response Guidebook. A Guide book for First Responders During the Initial Phase of a Dangerous Goods/Hazardous Materials Incident. Washington, D.C. 2004G-115]
 8. /GUIDE 115: GASES – FLAMMABLE (INCLUDING REFRIGERATED LIQUIDS)/ First Aid: Move victim to fresh air. Call 911 or emergency medical service. Give artificial respiration if victim is not breathing. Administer oxygen if breathing is difficult. Remove and isolate contaminated clothing and shoes. Clothing frozen to the skin should be thawed before being removed. In case of contact with liquefied gas, thaw frosted parts with lukewarm water. In case of burns, immediately cool affected skin for as long as possible with cold

water. Do not remove clothing if adhering to skin. Keep victim warm and quiet. Ensure that medical personnel are aware of the material(s) involved and take precautions to protect themselves. [QC reviewed] [U.S. Department of Transportation. 2004 Emergency Response Guidebook. A Guide book for First Responders During the Initial Phase of a Dangerous Goods/Hazardous Materials Incident. Washington, D.C. 2004G-115]

FLAMMABLE PROPERTIES ▲

Fire Potential:

SEVERE, WHEN EXPOSED TO HEAT OR FLAME. [Peer reviewed] [Sax, N.I. Dangerous Properties of Industrial Materials. 4th ed. New York: Van Nostrand Reinhold, 1975., p. 839]

NFPA Hazard Classification:

1. Health: 1. 1= Materials that, on exposure, would cause irritation, but only minor residual injury, including those requiring the use of an approved air-purifying respirator. These materials are only slightly hazardous to health and breathing protection is needed. [QC reviewed] [Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 325-61]
2. Flammability: 4. 4= Includes flammable gases, pyrophoric liquids, and Class IA flammable liquids. The preferred method of fire attack is to stop the flow of material or to protect exposures while allowing the fire to burn itself out. [QC reviewed] [Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 325-61]
3. Reactivity: 0. 0= Includes materials that are normally stable, even under fire exposure conditions, and that do not react with water. Normal fire fighting procedures may be used. [QC reviewed] [Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 325-61]

Flammable Limits:

LOWER 1.8%; UPPER 8.4% [QC reviewed] [Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 325-61]

Autoignition Temperature:

860 DEG F (460 DEG C) [QC reviewed] [Fire Protection Guide to Hazardous Materials. 12 ed. Quincy, MA: National Fire Protection Association, 1997., p. 325-61]

FIRE FIGHTING INFORMATION ▲

Fire Fighting Procedures:

1. CARBON DIOXIDE, DRY CHEM OR WATER SPRAY... [Peer reviewed] [Sax, N.I. Dangerous Properties of Industrial Materials. 4th ed. New York: Van Nostrand Reinhold, 1975., p. 839]
2. If material on fire or involved in fire: Do not extinguish fire unless flow can be stopped. Use water in flooding quantities as fog. Cool all affected containers with flooding quantities of water. Apply water from as far a distance as possible. [Peer reviewed] [Association of American Railroads. Emergency Handling of Hazardous Materials in Surface Transportation. Washington, DC: Association of American Railroads, Bureau of Explosives, 1994., p. 599]

3. Evacuation: If fire becomes uncontrollable or container is exposed to direct flame – consider evacuation of one-half (1/2) mile radius. [Peer reviewed] [Association of American Railroads. Emergency Handling of Hazardous Materials in Surface Transportation. Washington, DC: Association of American Railroads, Bureau of Explosives, 1994., p. 599]

Explosive Limits and Potential:

1. SEVERE, WHEN EXPOSED TO HEAT OR FLAME. [Peer reviewed] [Sax, N.I. Dangerous Properties of Industrial Materials. 4th ed. New York: Van Nostrand Reinhold, 1975., p. 839]
2. EXPLOSIVE LIMITS: LOWER 1.9%; UPPER 8.5% [Peer reviewed] [Sax, N.I. Dangerous Properties of Industrial Materials. 4th ed. New York: Van Nostrand Reinhold, 1975., p. 839]

HAZARDOUS REACTIONS ▲

Reactivities and Incompatibilities:

Strong oxidizers (eg, nitrates & perchlorates), chlorine, fluorine, (nickel carbonyl + oxygen). [QC reviewed] [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 176]

PREVENTIVE MEASURES ▲

Protective Equipment and Clothing:

1. Wear appropriate personal protective clothing to prevent the skin from becoming frozen from contact with the liquid or from contact with vessels containing the liquid. [QC reviewed] [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 176]
2. Wear appropriate eye protection to prevent eye contact with the liquid that could result in burns or tissue damage from frostbite. [QC reviewed] [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 176]
3. Quick drench facilities and/or eyewash fountains should be provided within the immediate work area for emergency use where there is any possibility of exposure to liquids that are extremely cold or rapidly evaporating. [QC reviewed] [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 176]
4. Personnel protection: ... Wear appropriate chemical protective gloves and goggles. [Peer reviewed] [Association of American Railroads. Emergency Handling of Hazardous Materials in Surface Transportation. Washington, DC: Association of American Railroads, Bureau of Explosives, 1994., p. 599]
5. Evacuation: ... If material leaking (not on fire) consider evacuation from downwind area based on amount of material spilled, location and weather conditions. [Peer reviewed] [Association of American Railroads. Emergency Handling of Hazardous Materials in Surface Transportation. Washington, DC: Association of American Railroads, Bureau of Explosives, 1994., p. 599]

Other Preventative Measures:

1. SRP: Local exhaust ventilation should be applied wherever there is an incidence of point source emissions or dispersion of regulated contaminants in the work area. Ventilation control of the contaminant as close to its point of generation is both the most economical and safest method to minimize personnel exposure to airborne contaminants. [Peer

- reviewed]
2. Work clothing that becomes wet should be immediately removed due to its flammability hazard. [QC reviewed] [NIOSH. NIOSH Pocket Guide to Chemical Hazards. DHHS (NIOSH) Publication No. 97-140. Washington, D.C. U.S. Government Printing Office, 1997., p. 176]
 3. If material not on fire and not involved in fire: Keep sparks, flames, and other sources of ignition away. Keep material out of water and sources and sewers. Attempt to stop leak if without undue personnel hazard. Use water spray to knock-down vapors. [Peer reviewed] [Association of American Railroads. Emergency Handling of Hazardous Materials in Surface Transportation. Washington, DC: Association of American Railroads, Bureau of Explosives, 1994., p. 599]
 4. Personnel protection: Avoid breathing vapors. Keep upwind. ... Do not handle broken packages unless wearing appropriate personal protective equipment. Approach fire with caution. [Peer reviewed] [Association of American Railroads. Emergency Handling of Hazardous Materials in Surface Transportation. Washington, DC: Association of American Railroads, Bureau of Explosives, 1994., p. 599]

OTHER SAFETY AND HANDLING ▲

Shipment Methods and Regulations:

1. No person may /transport,/ offer or accept a hazardous material for transportation in commerce unless that person is registered in conformance ... and the hazardous material is properly classed, described, packaged, marked, labeled, and in condition for shipment as required or authorized by ... /the hazardous materials regulations (49 CFR 171-177)./ [QC reviewed] [49 CFR 171.2; U.S. National Archives and Records Administration's Electronic Code of Federal Regulations. Available from: <http://www.gpoaccess.gov/ecfr/> as of February 15, 2006]
2. The International Air Transport Association (IATA) Dangerous Goods Regulations are published by the IATA Dangerous Goods Board pursuant to IATA Resolutions 618 and 619 and constitute a manual of industry carrier regulations to be followed by all IATA Member airlines when transporting hazardous materials. [QC reviewed] [International Air Transport Association. Dangerous Goods Regulations. 47th Edition. Montreal, Quebec Canada. 2006., p. 205]
3. The International Maritime Dangerous Goods Code lays down basic principles for transporting hazardous chemicals. Detailed recommendations for individual substances and a number of recommendations for good practice are included in the classes dealing with such substances. A general index of technical names has also been compiled. This index should always be consulted when attempting to locate the appropriate procedures to be used when shipping any substance or article. [QC reviewed] [International Maritime Organization. International Maritime Dangerous Goods Code. London, UK. 2004., p. 95]

Storage Conditions:

WHERE THESE SUBSTANCES ARE STORED & USED, PRECAUTIONS MUST BE PROVIDED TO PREVENT INJURY FROM FIRE & EXPLOSION & TO PREVENT INJURY TO HEALTH. /ALIPHATIC HYDROCARBONS/ [Peer reviewed] [International Labour Office. Encyclopedia of Occupational Health and Safety. Volumes I and II. New York: McGraw-Hill Book Co., 1971., p. 688]

Cleanup Methods:

The efficiency of any soil venting operation will depend significantly on three factors: vapor flowrate, vapor flow path relative to the contaminant distribution, and

composition of the contaminant. Simple mathematical models were developed to be used as screening tools to help determine if soil venting will be a viable remediation option at any given spill site. The models relate the applied vacuum, soil permeability, and spill composition to the vapor flowrates, velocities, mass removal rates, and residual composition changes with time. In this report the screening models and some sample calculations are presented. The results illustrate the advantages and limitations of venting as a remediation tool, under both ideal and nonideal conditions. [Peer reviewed] [Johnson PC; Ground Water 28 (3): 413-29 (1990)]

Disposal Methods:

SRP: At the time of review, criteria for land treatment or burial (sanitary landfill) disposal practices are subject to significant revision. Prior to implementing land disposal of waste residue (including waste sludge), consult with environmental regulatory agencies for guidance on acceptable disposal practices. [Peer reviewed]

5.0 TOXICITY/BIOMEDICAL EFFECTS

TOXICITY EXCERPTS ▲

Human Toxicity Excerpts:

1. Human volunteers exposed to 2500 to 1000 ppm for 1 min to 8 hr and 500 ppm for 1 to 8 hr/day for 10 days showed no deleterious effects. [Peer reviewed] [Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 3183]
2. Toxicologically, the vapor exerts no effect on skin and eyes, except as a liquid in direct contact, where it produces chemical burns. [Peer reviewed] [Clayton, G. D. and F. E. Clayton (eds.). Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 3183]
3. LOWER MEMBERS...GASES OF LOW ANESTHETIC POTENCY. /ALIPHATIC HYDROCARBONS/ [Peer reviewed] [Gosselin, R.E., H.C. Hodge, R.P. Smith, and M.N. Gleason. Clinical Toxicology of Commercial Products. 4th ed. Baltimore: Williams and Wilkins, 1976., p. II-103]
4. EXPOSURES TO ISOBUTANE (250, 500, OR 1000 PPM) FOR PERIODS OF 1 MIN-8 HR PRODUCED NO UNTOWARD PHYSIOLOGICAL EFFECTS AS DETERMINED BY METHODS WHICH INCL SERIAL EKG'S & CONTINUOUS MONITORING OF MODIFIED V5 BY TELEMETRY. [Peer reviewed] [STEWART ET AL; ENVIRON HEALTH PERSPECT 26 278-85 (1978)]
5. NO UNTOWARD EFFECTS WERE OBSERVED IN EIGHT ADULTS, MALES & FEMALES, EXPOSED TO 250-1000 PPM IN CONTROLLED-ENVIRONMENT CHAMBER FOR PERIODS OF 1 MIN, 2 MIN, 1 HR, 2 HR & 8 HR. ALSO NO UNTOWARD EFFECTS OCCURRED AFTER CHRONIC EXPOSURES TO 500 PPM. [Peer reviewed] [STEWART ET AL; SCAND J WORK ENVIRON HEALTH 3 (4): 234-43 (1977)]
6. AFTER EXPOSURES TO AEROSOL PROPELLANTS IN GREATER CONCEN THAN THOSE ENCOUNTERED IN NORMAL DOMESTIC USES, NOT ANY OF THOSE EXPOSED SHOWED ANY DECREMENT IN PULMONARY FUNCTION OR ALTERATION IN CARDIAC RHYTHM. [Peer reviewed] [STEWART ET AL; ENVIRON HEALTH PERSPECT 26: 275-85 (1978)]

Non-Human Toxicity Excerpts:

1. ALL 7 PROPELLANTS, WHICH INCL ISOBUTANE, CAUSED APNEA & FINALLY CARDIAC ARREST IN ANESTHETIZED RATS. [Peer reviewed] [FRIEDMAN ET AL;

- TOXICOL 1 (4): 345-55 (1973)]
2. At high concentrations it caused a decrease in pulmonary compliance and tidal volume in the rat. [Peer reviewed] [Clayton, G. D. and F. E. Clayton (eds.). *Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology*. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 3183]
 3. ... The anesthetized dog showed no significant effects up to 2 percent, but decreased myocardial contractility at 2.5 percent, exaggerated effects at 5 percent, with a decrease in ventricular and aortic pressure, and at 10 percent decreased left ventricular pressure, mean arterial flow, and stroke volume, with increased pulmonary vascular resistance. [Peer reviewed] [Clayton, G. D. and F. E. Clayton (eds.). *Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology*. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 3183]
 4. In the mouse, isobutane is a /CNS depressant/ at 15 percent in 60 min, and at 23 percent in 26 min. At 22 to 27 percent it is anesthetic in the mouse in 8.7 min, but caused respiratory arrest in 15 min. [Peer reviewed] [Clayton, G. D. and F. E. Clayton (eds.). *Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology*. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 3184]
 5. In the dog, anesthesia occurs at 45 percent in 10 min. [Peer reviewed] [Clayton, G. D. and F. E. Clayton (eds.). *Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology*. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 3184]
 6. Ninety-day inhalation studies were conducted on 50:50 weight percent (wt %) mixtures of n-butane, n-pentane, and isobutane, isopentane, respectively, and on a distillation cut boiling below 145 deg F of a reference unleaded gasoline blend to assess the nephrotoxicity of these volatile mixtures. The mixtures of butanes and pentanes were selected because these four hydrocarbons are the most prevalent components of gasoline vapors encountered under typical occupational exposures. The 0-145 deg F gasoline distillation fraction was tested because it reasonably approximates the composition of gasoline vapors measured under occupational settings. Male and female F-344 rats were exposed to 2 levels of each mixture, 6 hr/day, 5 days/wk, for 13 weeks. The target concentrations for the butane:pentane mixtures were 4500 and 1000 ppm, while 5200 and 1200 ppm were set for the gasoline distillation fraction. An interim sacrifice was conducted after 28 days. The rats were not significantly affected by the exposures, and there was no evidence of hydrocarbon-induced nephropathy in either sex at the termination of each study. However, at the 28-day interim sacrifice period for both butane:pentane mixtures, mild, transient treatment-related but not exposure-related kidney effects were observed in the male rats. These perturbations were absent at the interim sacrifice period for the gasoline distillation fraction. [Peer reviewed] [Aranyi C et al; *Toxicol Ind Health* 2 (1): 85-98 (1986)]
 7. The nephrotoxicity of 4 and 5 carbon containing gasoline components was studied in rats. Sprague-Dawley rats were exposed to a blend containing 25% (weight/weight) each of n-butane, n-pentane, isobutane, and isopentane by inhalation at concentrations of 0, 44, 432, or 4,437 ppm for 6 hr/day, 5 days/wk for 3 weeks. The animals were observed for clinical signs of toxicity. At the end of the study period, the rats were killed and necropsied. Blood was collected from the abdominal aorta for hematologic and serum chemistry analysis. No clinical signs of toxicity were seen. No gross or histopathological lesions were noted and no evidence of nephrotoxicity was observed. All hematologic and clinical chemistry parameters were within normal limits. The authors note that the 4,437 ppm exposure approaches 30% of the lower explosive limit of the hydrocarbon blend. They conclude that the four hydrocarbons do not appear to be nephrotoxic. It is possible that exposure to gasoline vapors in the workplace or in the consumer may not pose a significant nephrotoxic hazard, since 4 and 5 carbon isomeric hydrocarbons constitute such a large proportion of gasoline vapor and since occupational exposure to gasoline vapors is relatively low. [Peer reviewed] [Halder CA et al; *American Industrial Hygiene Association Journal* 47 (3): 173-5 (1986)]

TOXICITY VALUES ▲

Non-Human Toxicity Values:

LC50 Mouse inhalation 52 mg/kg for 1 hr exposure. [Peer reviewed] [Clayton, G. D. and F. E. Clayton (eds.). *Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology*. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 3183]

Populations at Special Risk:

Monitoring surveys of gasoline vapor exposures were conducted on truck drivers and terminal operators from 5 terminal loading facilities, on dockmen and seamen at 2 ship loading facilities and on attendants at 1 gas service station. Respective 8 hr TWA geometric mean exposures were 1.4 ppm at the terminal and 1 ppm at the gas station. The geometric mean exposures to benzene contained in gasoline vapors was 0.3 ppm for terminal workers and 0.2 ppm for the marine terminals and the gas station workers. Analysis of the composition of gasoline vapors revealed that C4 and C5 hydrocarbons constituted anywhere from 67 to 74% by weight of a typical vapor. 90% of this fraction was composed of n-butane, isobutane, n-pentane and isopentane. A short-term 21 day inhalation study on rats exposed to a blend of these 4 hydrocarbons was conducted to assess the potential for these major gasoline vapor components to induce kidney damage. No evidence of lesion was observed in rats exposed at up to 4437 ppm of the blend. [Peer reviewed] [Halder CA et al; *American Industrial Hygiene Association Journal* 47 (3): 164-75 (1986)]

PHARMACOKINETICS ▲

Metabolism/Metabolites:

Isobutane is oxidatively metabolized by rat liver microsomes to its parent alcohol. [Peer reviewed] [Clayton, G. D. and F. E. Clayton (eds.). *Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology*. 3rd ed. New York: John Wiley Sons, 1981-1982., p. 3184]

7.0 ENVIRONMENTAL FATE/EXPOSURE POTENTIAL

SUMMARY ▲

Environmental Fate/Exposure Summary:

Isobutane is a component of petroleum and natural gas and may be released as evaporative emissions or in wastewater resulting from the manufacture, storage and distribution of gasoline. It is also released in vehicle exhaust. Consumer products may contain isobutane which will be release to the atmosphere when these products are used. Isobutane is estimated to have a very low adsorptivity to soil. Since isobutane is a gas and has very high Henry's Law constant and low adsorptivity to soil, it would be expected to rapidly volatilize from moist and dry soil. Isobutane is biodegradable, especially when acclimated, and may also biodegrade in soil. If released in water, isobutane would readily volatilize; estimated half-lives for a model river and model lake are 2.2 hr and 3.0 days, respectively. Microcosm

experiments designed to replicate conditions in Narragansett Bay, RI indicate that volatilization will be the dominant removal mechanism for isobutane from the water column following a hypothetical input. Its volatilization half-lives in natural estuaries are estimated to be 4.4 and 6.8 days at 20 and 10 deg C, respectively. Isobutane also biodegrades in the microcosm with an initial rate commensurate with half-lives of 16–26 days at 20 deg C, significantly slower than the loss predicted by gas exchange. However, after acclimation of 2–4 weeks, the biodegradation rate increases markedly so that in the case of continuous environmental releases, biodegradation may become the dominant removal mechanism. Isobutane is not expected to bioconcentrate in aquatic organisms. Isobutane is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is 6.9 days. People are exposed to isobutane in ambient air, especially in areas of high traffic and at service stations, as well as by dermal contact with petroleum products. (SRC) [Peer reviewed]

POLLUTION SOURCES ▲

Natural Occurring Sources:

1. RAW NATURAL GAS/CONTAINS AVG/0.35 mol% ISOBUTANE [Peer reviewed] [Kirk-Othmer Encyclopedia of Chemical Technology. 3rd ed., Volumes 1–26. New York, NY: John Wiley and Sons, 1978–1984., p. V12 911]
2. Isobutane naturally occurs in petroleum and natural gas(3). From its Henry's Law Constant and atmospheric concns over the ocean, oceans appear to be supersaturated with isobutane by 2–3 orders of magnitude indicating that they are a source of isobutane (1,2). However oceans appear to be a minor source of alkanes compared with continental production(2). The flux of isobutane estimated for the mid-Atlantic between 35 deg N and 30 deg S is 0.32×10^8 molec/sq cm-sec(1). [Peer reviewed] [(1) Plass C et al; J Atmos Chem 15: 235–51 (1992) (2) Bonsang B et al; J Atmos Chem 6: 3–20 (1988) (3) Fujita EM et al; Environ Sci Technol 28: 1633–49 (1994)]

Artificial Sources:

1. Isobutane is found in gasoline and commercial gas(3) and may be released to the environment in evaporative losses, wastewater, and spills(SRC) as well as in combustion exhaust(3). Composition profiles for isobutane in auto emissions acquired using Federal Test Procedure tests include: USEPA 46 in-use vehicles for 1975–1982 model years, 0.92 wt%; Auto/Oil Program older (1983–1985) vehicle fleet, 0.21 wt%(3). Emissions of 25 vehicles (mostly 1986 model year) were tested under different driving conditions(1). The average emission were (type of driving (avg speed), emissions in mg/km): cold start (18.51 km/hr), 75.01; warm start (18.53 km/hr), 95.68; urban (21.38 km/hr), 65.66; suburban (41.73 km/hr), 29.64; rural (54.53 km/hr), 17.44; motorway (90.72 km/hr), 8.81; motorway (111.36 km/hr), 8.57(1,2). For suburban driving, 4 low emission vehicles had isobutane emissions of 0.8–18 mg/kg(2). The emission of isobutane from a car dropped from 53 mg/km at 20 km/hr to 9 mg/km between 90 and 110 km/hr(1). In emission tests using single component fuels, isobutane occurred in engine emissions when n-heptane, 1-hexene, and cyclohexane was burned, but not with toluene, isooctane or methyl tert-butyl ether (MTBE)(4). [Peer reviewed] [(1) Bailey JC et al; Atmos Environ 24A: 43–52 (1990) (2) Bailey JC et al; Sci Total Environ 93: 199–206 (1990) (3) Fujita EM et al; Environ Sci Technol 28: 1633–49 (1994) (4) Siegl WO et al; J Air Waste Manage Assoc 42: 912–20 (1992)]
2. Isobutane emission rates for the California South Coast Air Basin is 12.1 metric tons/day (6). A study of VOC emission in California South Coast Air Basin found that the sources of isobutane were (source, percent): gasoline exhaust, 6%; whole gasoline, 3%; gasoline vapors, 36%; waste and natural gas, 21%; 34%, other(5). No isobutane emissions were

attributed to coatings and adhesives(5). Isobutane gasoline exhaust emissions in the U.K have been estimated to be 5.29 and 14.5 kilotonnes by two investigators, constituting respectively 2% and 4% of exhaust emissions(1,3). Isobutane is found in underwater hydrocarbon vent plumes from offshore production; the concn in one plume was 560 umol/l(7). Isobutane constituted 0.004% of municipal sanitary landfill gas at Palos Verdes, CA(2). The landfill was in the anaerobic phase. Isobutane was found in emissions from the combustion of waste PVC plastics under conditions of incomplete combustion but not under conditions of complete combustion(4). Isobutane is used in consumer products such as insect spray, window and glass cleaner, personal spray deodorant, and rug and upholstery cleaners(8) and may be released when these products are manufactured or used(SRC). [Peer reviewed] [(1) Field RA et al; Atmos Environ 26A: 2983-96 (1992) (2) Brousseau J, Heitz M; Atmos Environ 28: 285-93 (1994) (3) Bailey JC et al; Atmos Environ 24A: 43-52 (1990) (4) Nishikawa H et al; Chemosphere 25: 1953-60 (1992) (5) Harley RA et al; Environ Sci Technol 26: 2395-408 (1992) (6) Grosjean D et al; Environ Sci Technol 27: 110-20 (1993) (7) Sauer TC Jr; Environ Sci Technol 15: 917-23 (1981) (8) USEPA; Compilation and speciation of national emissions factors for consumer/commercial solvent use information compiled to support urban air toxics assessment studies. USEPA/450/2-89/008, PB89-2072031 (1989)]

ENVIRONMENTAL FATE ▲

1. **TERRESTRIAL FATE:** Based on a recommended classification scheme(1), an estimated Koc value of 35(SRC), derived from a molecular structure estimation method(2) suggests that isobutane will have very high mobility in soil(SRC). Its very high Henry's Law constant, 4.08 atm-cu m/mole(SRC), (calculated from its vapor pressure(3) and water solubility(5)), high vapor pressure, 2611 mm Hg at 25 deg C(3), and low adsorptivity to soil indicate that volatilization will be an important fate process from both moist and dry soil surfaces(4, SRC). Isobutane is biodegradable, especially under acclimated conditions(6,7), and may biodegrade in soil. [Peer reviewed] [(1) Swann RL et al; Res Rev 85: 23 (1983) (2) Meylan WM et al; Environ Sci Technol 28: 459-65 (1992) (3) Riddick JA et al; Organic Solvents 4th ed NY, NY: Wiley (1986) (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods, NY: McGraw-Hill Chapt 16 (1982) (5) McAuliffe C; J Phys Chem 70: 1267-75 (1966) (6) Hou CT et al; Appl Environ Microbiol 46: 178-84 (1983) (7) Bopp RF et al; Org Geochem 3: 9-14 (1981)]
2. **AQUATIC FATE:** Based on a recommended classification scheme(1), an estimated Koc value of 35(SRC), determined from molecular structure(2), indicates that isobutane would not adsorb to sediment and particulate matter in the water column(SRC). Additional evidence that isobutane is not removed to sediment has been obtained from microcosm experiments(7). Isobutane will readily volatilize from water based on its estimated Henry's Law constant of 4.08 atm-cu m/mole(SRC), calculated from its vapor pressure(3) and water solubility(8). Estimated half-lives for a model river and model lake are 2.2 hr and 3.0 days, respectively(4, SRC). An estimated BCF value of 74(4, SRC), based on a log Kow of 2.76(5), suggests that isobutane will not bioconcentrate in aquatic organisms(SRC), according to a recommended classification scheme(6). [Peer reviewed] [(1) Swann RL et al; Res Rev 85: 23 (1983) (2) Meylan WM et al; Environ Sci Technol 28: 459-65 (1992) (3) Riddick JA et al; Organic Solvents 4th ed; NY, NY: Wiley (1986) (4) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Chapt 5, 15 (1982) (5) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (6) Franke C et al; Chemosphere 29: 1501- 14 (1994) (7) Bopp RF et al; Org Geochem 3: 9-14 (1981) (8) McAuliffe C; J Phys Chem 70: 1267-75 (1966)]
3. **AQUATIC FATE:** Experiments performed with gaseous C2-C4 alkanes in a microcosm designed to replicate Narragansett Bay, RI in September (20 deg C) and November (10 deg C) have shown that the removal rate of isobutane is 0.061/day (standard deviation

0.005/day) at 20 deg C and 0.030/day (standard deviation 0.006/day) at 10 deg C(1). The respective half-lives are 11 days and 23 days (SRC). The results indicate that gas exchange is the dominant removal mechanism for isobutane gases from the water column following a hypothetical input. Scaling up the predicted gas exchange rates (0.26/day and 0.017/day at 20 and 10 deg C, respectively(1)) so they are consistent with natural estuaries(1), the volatilization half-lives for isobutane from the water columns in natural estuaries(1) are estimated to be 4.4 and 6.8 days at 20 and 10 deg C, respectively (SRC). Isobutane also biodegrades in the microcosm at a rate that is slower than for n-butane and falls between propane and ethane in susceptibility. Biodegradation of isobutane initially occurs with a half-lives of 16–26 days at 20 deg C and 33–139 days at 10 deg C (1), significantly slower than the loss predicted by gas exchange from typical natural estuaries. However, after a lag of 2–4 weeks, the biodegradation rate increases markedly so that in the case of chronic inputs, biodegradation can become the dominant removal mechanism(1). [Peer reviewed] [(1) Bopp RF et al; *Org Geochem* 3: 9–14 (1981)]

4. **ATMOSPHERIC FATE:** Isobutane is a gas at ordinary temperatures, having a vapor pressure of 2611 mm Hg at 25 deg C(1). It is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is 6.9 days, assuming a hydroxyl radical concn of 5×10^5 radicals per cubic cm(2,SRC). When isobutane was exposed to sunlight for 6 hr in a tedlar bag filled with Los Angeles air, 6% of the isobutane degraded(3). The air contained 4529 ppb-C hydrocarbons and 870 ppb of NOX. The tropospheric loss of volatile hydrocarbons such as isobutane by wet and dry deposition are believed to be of minor importance(4). Indeed, isobutane assimilated into precipitation may evaporate during transport as well as being reemitted into the atmosphere after deposition(4). Isobutane is a contributor to the production of PAN (peroxyacyl nitrates) under photochemical smog conditions(5,6). [Peer reviewed] [(1) Riddick JA et al; *Organic Solvents* 4th ed; NY, NY: Wiley (1986) (2) Atkinson R; *J Chem Phys Ref Data Monograph* 1 (1989) (3) Kopczynski SL et al; *Environ Sci Technol* 6: 342–7 (1972) (4) Field RA et al; *Atmos Environ* 26A: 2983–96 (1992) (5) Grosjean D et al; *Environ Sci Technol* 27: 110–20 (1993) (6) Altshuller AP; *Air Waste* 43 1221–30 (1993)]

ENVIRONMENTAL TRANSFORMATIONS ▲

Biodegradation:

Indigenous soil microorganisms will biodegrade petroleum products under aerobic conditions(1). Biodegradation may occur under anaerobic conditions at a much slower rates, particularly by sulfur-reducing bacteria(2). It was demonstrated that isobutane is oxidized by bacteria as the sole source of carbon and energy(1). The bacteria was isolated from lake water and soil near a refinery in New Jersey. In the case of a *Brevibacterium* sp., the rate of oxidation of isobutane was about 70% that of n-butane. However, no isobutane degraded in 8 days when incubated with groundwater contaminated with gasoline(3). Isobutane was subject to biodegradation in a microcosm designed to simulate conditions in Narragansett Bay, RI in September and November(4). The biodegradation half-lives for isobutane were 16–26 days for September (20 deg C) and 33–139 days for November (10 deg C)(4). The degradation rate was slower than for n-butane and fell between that of propane and ethane. The biodegradation increased markedly on acclimation. Approximately 95% of the isobutane present in the microcosm after 12.9 days degraded within the next 2 days(1). [Peer reviewed] [(1) Hou CT et al; *Appl Environ Microbiol* 46: 178–84 (1983) (2) Corapcopglu MY, Hossian MA; *J Theoret Biol* 142: 503–16 (1990) (3) Jamison VW et al; pp. 187–96 in *Proc Int Biodeg Symp 3rd Sharpley JM, Kaplan AM, eds Essex, England (1976)* (4) Bopp RF et al; *Org Geochem* 3: 9–14 (1981)]

Abiotic Degradation:

The rate constant for the reaction of isobutane with photochemically produced hydroxyl radicals is 2.34×10^{-12} cu cm/molecule-sec at 25 deg C(1). This corresponds to an atmospheric half-life of 6.9 days at an atmospheric concn of 5×10^5 hydroxyl radicals per cu cm(SRC). The reaction product, 2-methylpropionaldehyde, may further react in the atmosphere to form peroxyacyl nitrates (PANs), phytotoxic components of photochemical smog(3,4). The rate constant for the reaction of isobutane with nitrate radicals during the night is 9.70×10^{-17} cu cm/molecule-sec at 23 deg C(5). This corresponds to an atmospheric half-life of 83 days at an atmospheric concn of 1×10^9 nitrate radicals per cu cm which is typical of the urban troposphere(SRC). The rate constant for the reaction of isobutane with ozone is 2.0×10^{-23} cu cm/molecule-sec at 25 deg C (2). This corresponds to an atmospheric half-life of 1600 years at an atmospheric concn of 7×10^{11} molecules of ozone per cu cm(SRC). [Peer reviewed] [(1) Atkinson R; J Chem Phys Ref Data Monograph 1 (1989) (2) Atkinson R, Carter WPL; Chem Rev 84: 437-70 (1984) (3) Altshuller AP; Air Waste 43: 1221-30 (1993) (4) Carter WPL; Air Waste 44: 881-99 (1994) (5) Atkinson R; Atmos Environ 24A: 1-41 (1990)]

ENVIRONMENTAL TRANSPORT ▲**Bioconcentration:**

A BCF of 74 was estimated for isobutane (SRC), using a log Kow of 2.76(1) and a recommended regression-derived equation(2). According to a recommended classification scheme(3), this BCF value suggests that isobutane has a low potential for bioconcentration in fish and aquatic organisms(SRC). [Peer reviewed] [(1) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods, NY: McGraw-Hill Chapt 5, Eqn 5-2 (1982) (3) Franke C et al; Chemosphere 29: 1501-14 (1994)]

Soil Adsorption/Mobility:

Using an estimation method based on molecular connectivity indices(1), the Koc for isobutane is estimated to be 35(SRC). According to a suggested classification scheme(2), this Koc value suggests that isobutane will have very high mobility in soil (SRC). [Peer reviewed] [(1) Meylan WM et al; Environ Sci Technol 28: 459-65 (1992) (2) Swann RL et al; Res Rev 85: 23 (1983)]

Volatilization from Soil/Water:

The Henry's Law constant for isobutane estimated from its vapor pressure, 2611 mm Hg at 25 deg C(1), and water solubility, 48.9 mg/l(2), is 4.08 atm-cu m/mol (SRC). Using this value for the Henry's Law constant, the volatilization half-life for isobutane in a model river 1 m deep flowing at 1 m/s with a wind speed of 3 m/s is estimated to be 2.2 hr(3,SRC). Similarly, the volatilization half-life of isobutane from a model lake 1 m deep, with a 0.05 m/s current and a 0.5 m/s wind is estimated to be 3.0 days(3,SRC). Isobutane's high vapor pressure, low adsorptivity to soil, and high Henry's Law constant indicates that volatilization from dry and moist soil should occur(SRC). Experiments have indicated that the rate of gas exchange in natural estuaries such as Narragansett Bay and San Francisco Bay are

approximately 6 times that measured in a microcosm designed to replicate conditions in Narragansett Bay, RI(5). Scaling up the experimentally-determined gas exchange rates for isobutane, 0.026/day at 20 deg C and 0.017/day at 10 deg C(5), the rate constant for gas exchange from the water columns in natural estuaries would be 0.16/day and 0.10/day, respectively (half-life 4.4 and 6.8 days)(SRC). For comparison, the ratio of air to water concn of isobutane (dimensionless Henry's constant) determined measurements made on a cruise in the Indian Ocean varied in time and place, ranging from 0.02-1.13 (4.9×10^{-4} to 2.8×10^{-2} atm-cu m/mol(SRC)), indicating that the sea is supersaturated with isobutane and sea air exchange is the controlling factor for volatilization(4). [Peer reviewed] [(1) Riddick JA et al; *Organic Solvents* 4th ed; NY, NY: Wiley (1986) (2) McAuliffe C; *J Phys Chem* 70: 1267-75 (1966) (3) Lyman WJ et al; *Handbook of Chemical Property Estimation Methods*, NY: McGraw-Hill Chapt 15, 16 (1982) (4) Bonsang B et al; *J Atmos Chem* 6: 3-20 (1988) (5) Bopp RF et al; *Org Geochem* 3: 9-14 (1981)]

ENVIRONMENTAL CONCENTRATIONS ▲

Water Concentrations:

1. DRINKING WATER: Isobutane was not present in the only sample of tap water analyzed in New Jersey as part of the USEPA Total Exposure Assessment Methodology (TEAM) study(1). [Peer reviewed] [(1) Wallace LA; *Toxicol Environ Chem* 12: 215-36 (1986)]
2. SURFACE WATER: The average (standard deviation) concn of isobutane in surface water of the mid-Atlantic (35 deg N to 30 deg S) in September/October 1988 was 2.7 (3.11) picomoles/l(1). The average isobutane concn was lower in the southern hemisphere; the concn between 35 deg N - 8 deg N, 8 deg N - 3 deg S, and 3 deg S and 30 deg S was 4.9, 2.9 and 1.2 picomoles/l, respectively. The concn of isobutane in surface water in the Indian Ocean (n=8) ranged from 0.12 to 1.78 nl/l(2). While the concn varied, the relative abundance of isobutane with respect to nonmethane hydrocarbons was practically constant(2). [Peer reviewed] [(1) Plass C et al; *J Atmos Chem* 15: 235-51 (1992) (2) Bonsang B et al; *J Atmos Chem* 6: 3-20 (1988)]

Effluents Concentrations:

1. In a comprehensive survey of wastewater from 4000 industrial and publicly owned treatment works (POTWs) sponsored by the Effluent Guidelines Division of the USEPA, isobutane was identified in discharges of the following industrial category (positive occurrences, median concn in ppb): petroleum refining (1; 102.6), plastics and synthetics (1; 109.7), oil and gas extraction (3; 16.2)(1). The highest effluent concn was 109.7 ppb in the plastics and synthetics industry(1). [Peer reviewed] [(1) Shackelford WM et al; *Analyt Chim Acta* 146: 15-27 (supplemental data) (1983)]
2. Vehicle exhaust contained 720 ppb isobutane(2). In a 1988 study in the U.K., the 6-car average concn of isobutane in exhaust gas was 8175 ppb(1). [Peer reviewed] [(1) Blake NJ et al; *J Geophys Res Atmos* 98D: 2851-64 (1993) (2) Field RA et al; *Atmos Environ* 26A: 2983-96 (1992)]

Sediment/Soil Concentrations:

Hydrocarbon gases are present in low concns in the upper 2 m of sediment from the shelf, slope and basin of the Bering Sea; the concn range of isobutane in the 19 core samples analyzed were 4 to 340 nl/l interstitial water, with a median of 9 nl/l (1). It is believed that these chemicals are derived from low temperature biological and chemical processes on the sea floor(1). [Peer reviewed] [(1) Kvenvolden KA, Redden GD; *Geochim Cosmochim Acta* 44: 1145-50 (1988)]

Atmospheric Concentrations:

1. The concn of isobutane in air is largely a result of vehicle emissions and will be particularly sensitive to factors such as the sampling duration, type of location, wind direction, and time of day(2). This is exemplified by the concn of isobutane in air at Riverside, CA (n=6, afternoon with a heavy haze), 5.2–10.4 ppb, compared with 0.2 ppb on a clear morning(3). Ambient air concns for isobutane in the National Ambient Volatile Organic Compounds data base (n = 887): mean 5.706 ppb, median 3.290 ppb, 25th percentile 1.728 ppb, 75th percentile 6.213 ppb(1). The median concn by type of site were (type, number of data points, concn): remote, 6, 0.158 ppb; rural, 36, 0.340 ppb; suburban, 223, 3.817 ppb; urban, 546, 3.275 ppb; source dominated, 56, 4.204 ppb(1). 4-Hour simultaneous air sampling on 15 days over a 3 month period in the summer of 1987 of an industrial, urban and suburban site in Chicago resulted in mean levels of 4.42, 2.16, and 2.12 ug/cu m, respectively(4). The concn of isobutane in Japan along the direction of air mass movement was 4.4 ppb in Yokohama, 1.3 ppb in Takasaki, and 1.5 ppb in Kuruzawa (5). The decrease in concn was attributed to photooxidation. [Peer reviewed] [(1) Shah JJ, Heyerdahl EK; National Ambient VOC Database Update USEPA 600/3-88/010 (1988) (2) Field RA et al; Atmos Environ 26A: 2983-96 (1992) (3) Bonsang B et al; J Atmos Chem 6: 3-20 (1988) (4) Scheff PA, Wadden RA; Environ Sci Technol 27: 617-25 (1993) (5) Satsumabayashi H et al; Atmos Environ 26A: 2835-44 (1992)]
2. RURAL/REMOTE: Diurnal variation in isobutane concn in North Pacific marine air was either minimal or absent(1). Indian ocean cruise (n=22) 0.03–0.29 ppb, median 0.11 ppb(2). Year long monitoring at Birkenes, a rural site in southern Norway (n=39) 55–1180 parts/trillion with a mean of 1.14 ppb(3). Maximum and minimums were in late Jan and Sept, respectively. Monitoring at rural sites reported in the literature ranged from 140–1700 parts/trillion(3). Germany: background station (10/83), 0.22 ppb; semirural site (3/84, n=5), 1.7 ppb, mean; remote continental site (n=3), 0.17–0.28 ppb(4). Upper Egypt desert (n=5) 0.11 ppb(4). [Peer reviewed] [(1) Carsey TP; Marine tropospheric hydrocarbons: An intercomparison exercise. Atlantic Oceanogr Metreorol Lab Natl oceanic Atmos Adm, Miami, FL Report 1991, NOAA-DR-ERL-AOML-21 PB91-223735 (1991) (2) Bonsang B et al; J Atmos Chem 6: 3-20 (1988) (3) Hov O et al; Atmos Environ: 25A: 1981-99 (1991) (4) Rudolph J, Khedim A; Int J Environ Anal Chem 290: 265-82 (1985)]
3. Concns of isobutane resulting from urban (n=34, interstate (n=35), and rural (n=7) driving was assessed in Raleigh, NC in the summer of 1988 using a 1983 and a 1987 model cars (1). The concn was measured at: (a) the driver's breathing zone, (b) a location mid-route 100–300 ft from the roadway, (c) the car roof, (d) the breathing zone of a pedestrian along the urban route. The concn of isobutane in ug/cu m was (location, median, mean, maximum): (a) in-vehicle, 0.5, 9.1, 281.7; (b) fixed site, 1.7, 3.9, 43.4; (c) car exterior, 0.2, 8.5, 56.0; (d) sidewalk, 6.4, 8.0, 22.0. The in-vehicle median concn was 9.0 ug/cu m for urban driving, 2.2 ug/cu m for rural driving, and below the detection limit for interstate driving. [Peer reviewed] [(1) Chan CC et al; Environ Sci Technol 25: 964-72 (1991)]
4. URBAN: Results of year-round sampling (24-hr samples every 6th day) of ambient air for isobutane at a representative site in Washington DC (3/90–3/91): 92.96% frequency, max 3.8 ppb, median 1.26 ppb, mean 1.4 ppb, SD 0.85 ppb(1). Concn of isobutane in 39 U.S. cities between 1984–1986 (n=836) in ppbC: median 14.9, 25th percentile 8.5, 75th percentile 23.5, min 1.2, max 647(5). The concn of isobutane in remote marine is 0.11 ppb and in Sydney, Australia (1979–80) and Hamburg, Germany (1986–87) 4.7 ppb(3) and 3.8 ppb(2), respectively. The concn of isobutane in Vienna, Austria (n=5, street with heavy traffic, 1.5 m above the ground) was 7.1 ppbC with a standard deviation of 3.9 ppbC(6). The results of air monitoring for isobutane at Harwell, England between Mar 1973 and Aug 1974 (n=63) was 0.37–3.58 ppb with a mean of 1.2 ppb(4). [Peer reviewed] [(1) Hendler AH, Crow WL; in Proc Annu Meet Air Waste Manage Assoc, 85th (Vol 2B), 92/75.05 (1992) (2) Field RA et al; Atmos Environ 26A: 2983-96 (1992) (3) Nelson PF, Quigley SM; Environ Sci Technol 16: 650-5 (1982) (4) Stephens ER, Burleson FR; J Air Pollut Control Assoc 17: 147-53 (1967) (5) Seila RL et al; Determination of C2 to C12 Ambient Air Hydrocarbons in 39 US cities, from 1984 through 1986 USEPA/600/S3-89/058 (1989) (6)

- Lanzerstorfer C, Puxbaum H; *Water Air Soil Pollut* 51: 345-55 (1990)]
- PERSONAL AIR: Isobutane was identified in 5 of 8 samples in New Jersey analyzed as part of the USEPA Total Exposure Assessment Methodology (TEAM) study(1). [Peer reviewed] [(1) Wallace LA; *Toxicol Environ Chem* 12: 215-36 (1986)]
 - PLUME: The concn of isobutane in a photochemical plume in London ranged from 1159-1857 ppb with a mean of 1506 ppb. The concns out of the plume and upwind were 240-811, and 132-141 ppb, respectively. The mean concn of isobutane in three other London plumes were 969, 4141 and 1940 ppb(1). [Peer reviewed] [(1) Blake NJ et al; *J Geophys Res Atmos* 98D: 2851-64 (1993)]

Other Environmental Concentrations:

- Industry average gasoline from the Auto/Oil program database contains 8.3% isobutane(6). The isobutane content of automobile-related sources in wt% (source, content): gasoline exhaust (nuncatalyzed), 0.2%; gasoline exhaust (catalyzed), 0.5%; unburned gas, 0.8%; headspace vapors, 0.5%(1). The isobutane content (ppbC%) of sources from the 1990 Atlanta Ozone Precursor Monitoring Study were (source, content): whole gas (weighted avg all octanes), 0.599; whole gas 87 octane, 0.56; whole gas 89 octane, 0.60; whole gas 92/93 octane, 0.70; headspace gas 24 deg C (all octanes), 5.13; headspace gas 32 deg C (all octanes), 4.63(2). A similar study in the Chicago area yielded isobutane emission profiles (wt%) as (source, content): regular gas, 6.17; mid-grade gas, 6.51; premium gas 9.53; hot soak emissions, 4.98; cold start emissions, 1.84(3). Composition profiles for isobutane acquired during the Southern California Air Quality Study in wt% include (source, content): commercial natural gas, 2.10; geogenic natural gas, 5.90; liquified petroleum gas (LPG), 0.20; diurnal evaporative emissions, 1.76; hot soak evaporative emissions, 0.60; running loss evaporative emissions, 1.69; summer gas, 0.75; winter gas, 2.10; summer gas headspace, 11.51; winter gas headspace, 17.40(4). Vapors from two brands of alkylate-based petroleum contained 18.9 and 44.8% isobutane, respectively(5). [Peer reviewed] [(1) Harley RA et al; *Environ Sci Technol* 26: 2395-408 (1992) (2) Conner TL et al; *J Air Waste Manage Assoc* 45: 383-94 (1995) (3) Doskey PV et al; *J Air Waste Manage Assoc* 42: 1437-45 (1992) (4) Fujita EM et al; *Environ Sci Technol* 28: 1633-49 (1994) (5) Oestermark U, Peterssom G; *Chemosphere* 25: 763-8 (1992) (6) Sawyer RF; *Environ Health Perspect* 101(Suppl 6): 5-12 (1994)]
- Isobutane was present in 6 of 10 insect sprays analyzed for VOC content by USEPA; when present it constituted 15.01 to 15.22 wt% of the product VOC(1). Isobutane was present in 5 of 16 window and glass cleaners analyzed for VOC content by USEPA; when present it constituted 0.82 to 45.47% (vol) of the product VOC(1). Isobutane was present in 2 of 3 personal spray deodorants analyzed for VOC content by USEPA; when present it constituted 77.23 and 96.94 wt% of the product VOC(1). Isobutane was present in 1 of 12 rug and upholstery cleaners analyzed for VOC content by USEPA; when present it constituted 96.77 wt% of the product VOC(1). A composite profile for window and glass cleaners developed by USEPA from composition data for 16 products contains 8.63 wt% isobutane(1). It was assumed that all products had an equal market share. [Peer reviewed] [(1) USEPA; *Compilation and speciation of national emissions factors for consumer/commercial solvent use information compiled to support urban air toxics assessment studies. USEPA/450/2-89/008, PB89-2072031 (1989)]*
- AIR COMPOSITION PROFILES: The isobutane content (ppbC%) of vehicle-related air samples from the 1990 Atlanta Ozone Precursor Monitoring Study were: roadway (n=9), 1.12; airport (n=11), 0.96; aircraft (n=2), 0.525(2). The roadway samples were collected along a busy interstate during morning rush hour in August. Other roadway emission profiles for isobutane in wt% are: Chicago, 1.93; Lincoln Tunnel, 1.78; Atlanta roadway, 1.26 (3). The Chicago profiles were taken on a confined parkway during rush hour. The ground level emissions 1 mi downwind from a refinery contained 1.85-22.42 wt%, mean 8.02 wt% isobutane(3). An earlier study reported refinery emission profiles as 1.64-5.63 wt% isobutane with a mean of 3.97 wt%(1). [Peer reviewed] [(1) Sexton K, Westberg H; *J Air Pollut Control Assoc* 29: 1149 (1979) (2) Conner TL et al; *J Air Waste Manage Assoc* 45: