U.S. Department of Transportation
Pipeline and Hazardous Materials Safety Administration

1200 New Jersey Ave, S.E.
Washington, D.C. 20590

JUN 19 2009

Mr. Lawrence D. Rutledge
Advance Asymmetrics, Inc.
213 East White Street
Millstadt, IL 62260-1543

Ref. No. 09-0119

Dear Mr. Rutledge:

This responds to your May 1, 2009 letter requesting an interpretation of your procedure for classifying and describing di-tert-Butyldicarbonate under the Hazardous Materials Regulations (HMR; 49 CFR Parts 171-180).

Under § 173.22, it is the shipper's responsibility to class and describe a hazardous material. This Office does not perform that function. Your analysis of the physical and chemical properties of di-tert-Butyldicarbonate and your procedure for determining the classification, packing group assignment, and appropriate shipping description provides for a reasonable conservative conclusion. Your understanding is correct that the material is a solid as defined in accordance with § 171.8 and should be described as a solid. However, we are concerned that using a shipping description that identifies the material as a solid when the material may be shipped as a liquid may not convey appropriate information to transport workers and emergency responders. To ensure that complete information concerning the material is provided, you may add the qualifying word "molten" to the shipping description in accordance with § 172.101(c)(16). Alternatively, you may include additional information on the shipping paper to indicate the material may be in a liquid state during the normal course of transportation. Note that when the authorized packaging associated with the shipping description for material is inappropriate for the physical state of the material during transport, § 172.101(i)(4) should be used to determine the appropriate packaging.

I hope this information is helpful. If you have further questions, please do not hesitate to contact this office.

Sincerely,

Charles E. Betts
Chief, Standards Development
Office of Hazardous Materials Standards

Der Kinderen
§172.101
Classification
09-0119

Advanced Asymmetrics, Inc.
213 East White Street • Millstadt, IL 62260-1543
Phone 1-618-476-7408 or 1-888-330-6324
Fax 1-618-476-7408 or 1-888-704-3133

Steve Hwang
Office of Hazardous Materials Safety
Pipeline and Hazardous Materials Safety Administration
Attn: PHH-10, U.S. Department of Transportation, East Building
1200 New Jersey Avenue, SE.
Washington, DC 20590-0001

1-May-2009

Dear Mr. Hwang:

I represent a small research chemicals supplier attempting to classify a chemical for shipping. We generally have no problems doing this, after which we double check our work by verifying our classification against the classifications in a number of other company's MSDSs. In this case however we have encountered a problem with this protocol and would like to receive an official interpretation on our classification procedure.

Attached please find four of our competitor's MSDSs for di-tert-Butyldicarbonate. As you will see, they have each classified the compound differently, as UN2929, UN2930, UN2811, and UN 1325. The difference is important to us as it will affect the container sizes which we can list and ship in our catalog. The normal procedure suggested to us is to simply accept our supplier's classification. In this case however, our supplier is the one who classifies the product a UN 1325 which is both the lowest hazard and, in our opinion, the least defensible classification. We are unable to obtain a clarification from them as they have discontinued this product.

Our problem with the classification arises from the fact that much of the data required for proper classification is not available at the exact physical conditions required for analysis. As a result, we have made calculations of the expected values by various means. We are unclear as to the exact extent to which such a calculation is permissable in making classification. We would like our analysis as provided below to be reviewed with particular note to the approximations and calculated physical and toxicological properties. We are most interested in an indication of whether these calculations and the conclusions derived from them may be considered valid. If so, we would appreciate some guidance as to the limits of these methods.

The enclosed MSDSs should have all the information required to evaluate our assignment procedure. Please note that the MSDS from Acros (Maybridge) appears to have two errors in it:

- First it reports of a vapor pressure of 0.5 mmHg at 37 °C. This value appears nowhere else that I can find and appears to be either a typo of the correct value of 57 °C or an error caused by copying their flash point temperature of 37 °C. The value of 56-57 °C at 0.5 mmHg is consistent across all other vendors and is consistent with a nomograph-based prediction from the value of 70 °C at 1 mm Hg reported in the Sigma MSDS. All other physical and hazard data is consistent across all MSDSs.

- Second it correctly reports a correct LC_{50} of 100 mg / m^3 / 4 hour then notes a 1 hour LC50 of 400 mg / m3 can be approximated. This appears to be twice the correct value according to the approximations allowed by regulation.

One problem for classification is that no boiling point or vapor pressure can be found for temperatures below 57 °C while classification requires this value at 20 °C. The required value was estimated in the following way:

- Known vapor pressures are 1 mm Hg (1.33 hPa) @ 70 °C (only a single reference) and 0.5 mm Hg @ 56 °C (which is used in almost everyone's MSDS). Determination of a boiling point/vapor pressure at 20 °C was calculated using the boiling point calculator at http://www.trimen.pl/witek/calculators/wrzenie.html.

- The calculator's validity was checked by using it to predict some known boiling points and enthalpies of vaporization and found to be correct within a few degrees of temperature or several percent on enthalpy of vaporization, values which are within the expected experimental error.

- The calculator is "unfriendly" regarding the number of decimal places provided. The mathematics however are such than if a 1000 times too large vapor pressure is input, a 1000 time too large vapor pressure will be output, however the calculator will in this case provide a larger number of significant figures in the result. All calculations were done in this way to obtain a sufficient number of significant figures, then double-checked by calculation using the "uninflated" values and found correct.

- Boiling point calculation involves three data points - the boiling point at two pressures and the enthalpy of vaporization. Knowledge of any two allows prediction of the other. Additionally knowledge of two boiling points allows prediction of a third.
  - Using the known boiling points at 57 °C and 70 °C, an enthalpy of vaporization of 46.5 kJ/mol and a vapor pressure of 0.062 mm Hg at 20 °C.
  - A calculated enthalpy of vaporization based on molecular modeling of 47.26 kJ/mol was located. Using the same calculator with this enthalpy for calibration and using the 56 °C boiling point provides a vapor pressure of 0.060 mm Hg at 20 °C.
  - A calculated vapor pressure based on molecular modeling of 0.049 mm Hg at 25 °C was also located. Using the enthalpy of 47.26 kJ/mol for calibration, this predicts a vapor pressure of 0.035 mm Hg at 20 °C.

- Therefore calculations involving a vapor pressure will be made using the highest (0.062 mm Hg) and the lowest (0.035 mm Hg) values and the worst-case assumed.

It is worth noting that the predictions of *ca.* 0.06 mm Hg are based on an assumption of a liquid/gas equilibrium. At 20 °C the product is in fact a solid and the vapor pressure may reasonably be expected to be less than this amount.

Two final complications need to be addressed before making the final assignment:

- The product melting point is 22-24 °C. Products melting above 20 °C are considered solids for classification purposes, therefore this product is a solid. If shipped at a

temperature above 22 °C, the proper shipping name should include the word "molten" (but for classification and labeling purposes is still considered a solid). Note however that the regulations require the *initial* melting point to be above 20 °C to be considered a solid. As the product ages and becomes impure, the melting point will depress and eventually fall into the liquid category. Therefore we must acknowledge that some shipments of this product may in fact be liquid according to this definition. Accordingly we will present two different classifications, depending on whether the given sample is to be considered a liquid or a solid.

- Inhalation hazards must be considered for dusts (as solids), mists/aerosols (as liquids) and and vapors (either form). Again, we will present independent classifications for both solid and liquid forms.

Our classification for this product is as follows. I regret that we are unable to provide citations to DOT regulations. All citations are to 50th Edition IATA (2009). I trust you have access to a cross reference to specific DOT regulations.

1) First the product is classified based on its flammability, in both the solid and liquid forms:

- The product has a flash point of 99 °F / 37 °C, a temperature at which it would be a liquid. This corresponds to PG III. Decomposition however leads to tert-butanol as a product which has a flash point of 11 °C and which, in sufficient quantity, could reduce the flash point to the extent that it met the requirements for PG II, an effect which would depend on the exact level of impurity. Until a flash point is measured on an defined impure sample, we will use a working classification of PG II based on the flammability characteristic when the product is a liquid by regulations.
- There is no appropriate information regarding the solid flammability tests. The product clearly does not meet the classification of PG I. Local tests and experience suggest the solid classification of PG III, however at our current level of experience we do not wish to rely on those tests. Again until more accurate tests are performed we will use a working classification of PG II based on the flammability characteristic when the product is a solid by regulations.

2) Oral (>5000 mg/kg) and dermal (>2000 mg/kg) toxicities imply no toxic hazard by those routes and are valid for both solid and liquid forms.

3) Inhalation hazard classification must consider both dust/mist and vapor. We have a citation for a LC_{50} of 100 mg / m^3 / 4 hour but can not find any note indicating whether it is a dust/mist or a vapor exposure. The calculated vapor pressure at 20 °C would produce a saturated vapor of 794 mg / m^3, nearly eight times this value. It is reasonable therefore to assume this is a vapor measurement. None-the-less, exposures will be considered for dust, mist, and vapor modes of inhalation exposure to provide an additional margin of safety by shipping based on the most restrictive result. 3.6.1.5.3.2 states that the hazard is to be calculated based on LC_{50} / 1 hour but when only the 4 hour number is available, it may be used after doubling. The available number of 100 mg / m^3 is a 4 hour exposure, so a working inhalation toxicity of 200 mg / m^3 shall be used.

4) According to 3.6.1.5.3 a solid compound need only be tested if at least 10% (by mass) of the total is likely to be dust. In this case, the compound is packaged as a melt then allowed to freeze before shipping. It is a single mass so there is no potential for any significant dust, even were the

container to be shattered. Therefore, inhalation toxicity by dust need not be considered. When the product is a solid, according to 3.6.1.5.3 its hazards as a liquid (i.e. Mist/aerosol) need not be considered.

5) According to 3.6.1.5.3 a liquid need only be tested if a mist or aresols is likely to be generated by leakage of the transport containment. In this case however the compound is shipped unpressurized. The vapor pressure is quite low (under 1/1000 of an atmosphere) so no mist or aerosol would be generated by boiling at the reduced pressure of a flight. Again, therefore, inhalation toxicity by mist need not be considered.

6) In the case of either a solid or a liquid however, inhalation hazard by vapor is equally valid. There are two tests, both of which must confirm the hazard for proper classification.

- IATA regulations ask for toxicity in terms of mL / m^3. Since we are dealing with vapors, I understand this to mean mL of compound in the vapor phase per cubic meter of air. Using Ideal Gas Law and assuming a temperature of 20 °C (specified by 3.6.1.5.3.2), 200 mg / m^3 is 22 mL of vapor. According to table 3.6.B, 22 < 1000, so this is PG I by that test.
- The value of V (see note 1 on p 106, below table 3.6.B) must also be calculated and compared to multiples of the LC_{50} vapor concentration. V for the two vapor pressures of 0.062 and 0.049 mm Hg are 81 and 64. Both of the V values are less than 10 x LC_{50}. Failure of this second test means the product is not PG II. The two values are between 37% and 29% of the required threshold which, given the closeness of the calibration points and multiple calculations, is judged to be more than an adequate margin for error and far higher than the calculation uncertainties.
- Additionally UN3384 requires the same LC_{50} and V thresholds as the PG I test, so this is also not a proper classification.
- The test for PG II only requires V be greater than LC_{50}. Both V values are greater than LC_{50} so on that measure our conclusion is PG II according to inhalation toxicity

Based on these considerations, our classification is UN2930, Toxic solid, Flammable, Organic, n.o.s., 6.1(4.1), Packing Group II in those cases where the product is sufficiently pure that its initial melting point is greater than 20 °C, and UN2930, Toxic liquid, Flammable, Organic, n.o.s., 6.1(3), Packing Group II in those cases where the product is sufficiently impure that its initial melting point is 20 °C or less.

Please let me know if you concur with this classification. If additional clarifications are required, I may be reached at 618-476-3920 or at larry@4chiral.com.

Best Regards,

Lawrence D. Rutledge
Advanced Asymmetrics, Inc.

MAYBRIDGE

Material Safety Data Sheet
Di-tert-butyl dicarbonate

MSDS# 68225

Section 1 - Chemical Product and Company Identification

MSDS Name:	Di-tert-butyl dicarbonate
Catalog Numbers:	18977-0000, 18977-0050, 18977-1000, 18977-5000, 19467-0000, 19467-0100, 19467-0250, 19467-0500, 19467-1000, 19467-5000, 61275-0100, 61275-0250, 61275-0500, 61275-1000, 61275-5000, SB01692DA, SB01692EA, SB01692EE, SB01692ZZ
Synonyms:	Di-tert-butyl pyrocarbonate; DIBOC; BOC anhydride.

Company Identification:	Maybridge Trevillett, Tintagel Cornwall, England PL34 0HW
For information in the US, call:	800-ACROS-01
For information in Europe, call:	+32 14 57 52 11
Emergency Number, Europe:	+32 14 57 52 99
Emergency Number US:	201-796-7100
CHEMTREC Phone Number, US:	800-424-9300
CHEMTREC Phone Number, Europe:	703-527-3887

Section 2 - Composition, Information on Ingredients

CAS#:	24424-99-5
Chemical Name:	Di-tert-butyl dicarbonate
%:	97+
EINECS#:	246-240-1

Hazard Symbols: T+

Risk Phrases: 11 26 36/37/38 43

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Danger! Flammable solid. May be fatal if inhaled. May cause sensitization by skin contact. Causes eye, skin, and respiratory tract irritation. Target Organs: Central nervous system, respiratory system, eyes, skin.

Potential Health Effects

Eye: Causes eye irritation.

Skin: May cause skin irritation. May be harmful if absorbed through the skin. May cause sensitization by skin contact.

Ingestion: May cause irritation of the digestive tract. May be harmful if swallowed.

Inhalation: May be fatal if inhaled. Causes respiratory tract irritation.

Chronic: Repeated or prolonged exposure may cause allergic reactions in sensitive individuals.

Section 4 - First Aid Measures

Eyes: Immediately flush eyes with plenty of water for at least 15 minutes, occasionally lifting the upper and lower eyelids. Get medical aid.

Skin: Get medical aid. Immediately flush skin with plenty of water for at least 15 minutes while removing contaminated clothing and shoes.

Ingestion: Do not induce vomiting. Get medical aid.

Inhalation: POISON material. If inhaled, get medical aid immediately. Remove victim to fresh air. If not breathing, give artificial respiration. If breathing is difficult, give oxygen.

Notes to Physician: Treat symptomatically and supportively.

Section 5 - Fire Fighting Measures

General Information: As in any fire, wear a self-contained breathing apparatus in pressure-demand, MSHA/NIOSH (approved or equivalent), and full protective gear. Vapors may form an explosive mixture with air. Vapors can travel to a source of ignition and flash back. Use water spray to keep fire-exposed containers cool. Containers may explode in the heat of a fire. Flammable solid.

Extinguishing Media: Use water spray to cool fire-exposed containers. Use foam, dry chemical, or carbon dioxide. Water may be ineffective.

Autoignition Temperature: 460 deg C (860.00 deg F)

Flash Point: 37 deg C (98.60 deg F)

Explosion Limits: Lower: Not available

Explosion Limits: Upper: Not available

NFPA Rating: health: 4; flammability: 3; instability: 1;

Section 6 - Accidental Release Measures

General Information: Use proper personal protective equipment as indicated in Section 8.

Spills/Leaks: Wear a self contained breathing apparatus and appropriate personal protection. (See Exposure Controls, Personal Protection section). Sweep up or absorb material, then place into a suitable clean, dry, closed container for disposal. Avoid generating dusty conditions. Remove all sources of ignition. Use a spark-proof tool. Do not let this chemical enter the environment.

Section 7 - Handling and Storage

Handling: Minimize dust generation and accumulation. Use spark-proof tools and explosion proof equipment. Do not get in eyes, on skin, or on clothing. Keep away from heat, sparks and flame. Do not ingest or inhale. Use only in a chemical fume hood.

Storage: Keep away from sources of ignition. Store in a tightly closed container. Store in a dry area. Flammables-area. Keep refrigerated. (Store below 4°C/39°F.)

Section 8 - Exposure Controls, Personal Protection

Chemical Name	ACGIH	NIOSH	OSHA - Final PELs
Di-tert-butyl dicarbonate	none listed	none listed	none listed

OSHA Vacated PELs: Di-tert-butyl dicarbonate: None listed

Engineering Controls:

Use explosion-proof ventilation equipment. Facilities storing or utilizing this material should be equipped with an eyewash facility and a safety shower. Use only under a chemical fume hood.

Exposure Limits

Personal Protective Equipment

Eyes: Wear appropriate protective eyeglasses or chemical safety goggles as described by OSHA's eye and face protection regulations in 29 CFR 1910.133 or European Standard EN166.

Skin: Wear appropriate protective gloves to prevent skin exposure.

Clothing: Wear appropriate protective clothing to prevent skin exposure.

Respirators: Follow the OSHA respirator regulations found in 29 CFR 1910.134 or European Standard EN 149. Use a NIOSH/MSHA or European Standard EN 149 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.

Section 9 - Physical and Chemical Properties

Physical State: Physical State:

Color: white

Odor: characteristic odor

pH: Not available

Vapor Pressure: 1.33 hPa @ 70 deg C

Vapor Density: Not available

Evaporation Rate: Not available

Viscosity: Not available

Boiling Point: 37 deg C @ 0.5 mmHg (98.60°F)

Freezing/Melting Point: 22 - 24 deg C

Decomposition Temperature: Not available

Solubility in water: Hydrolysis.

Specific Gravity/Density: 1.020

Molecular Formula: C10H18O5

Molecular Weight: 218.25

Section 10 - Stability and Reactivity

Chemical Stability:	Moisture sensitive.
Conditions to Avoid:	Incompatible materials, ignition sources, dust generation, excess heat, exposure to moist air or water.
Incompatibilities with Other Materials	Reducing agents, acids, bases.
Hazardous Decomposition Products	Carbon monoxide, carbon dioxide, n-butanol, isobutylene.
Hazardous Polymerization	Will not occur.

Section 11 - Toxicological Information

RTECS#: CAS# 24424-99-5: HT0230000

LD50/LC50: RTECS:

CAS# 24424-99-5: Inhalation, rat: LC50 = 100 mg/m3/4H;

Other: One hour LC50 can be approximated as 400 mg/1000 liter or .4 mg/liter.

Carcinogenicity: Di-tert-butyl dicarbonate - Not listed as a carcinogen by ACGIH, IARC, NTP, or CA Prop 65.

Epidemiology: No information found

Teratogenicity: No information found

Reproductive: No information found

Neurotoxicity: No information found

Mutagenicity: No information found

Other: See actual entry in RTECS for complete information.

Section 12 - Ecological Information

Other: Do not empty into drains.

Section 13 - Disposal Considerations

Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. US EPA guidelines for the classification determination are listed in 40 CFR Parts 261.3. Additionally, waste generators must consult state and local hazardous waste regulations to ensure complete and accurate classification. RCRA P-Series: None listed. RCRA U-Series: None listed.

Section 14 - Transport Information

US DOT
Shipping Name: TOXIC SOLIDS, FLAMMABLE, ORGANIC, N.O.S.
Hazard Class: 6.1
UN Number: UN2930
Packing Group: I
Canada TDG
Shipping Name: TOXIC SOLIDS, FLAMMABLE, ORGANIC, N.O.S.
Hazard Class: 6.1
UN Number: UN2930
Packing Group: I

Section 15 - Regulatory Information

US Federal

TSCA

CAS# 24424-99-5 is listed on the TSCA Inventory.

Health & Safety Reporting List	None of the chemicals are on the Health & Safety Reporting List.
Chemical Test Rules	None of the chemicals in this product are under a Chemical Test Rule.
Section 12b	None of the chemicals are listed under TSCA Section 12b.
TSCA Significant New Use Rule	None of the chemicals in this material have a SNUR under TSCA.
CERCLA Hazardous Substances and corresponding RQs	None of the chemicals in this material have an RQ.
SARA Section 302 Extremely Hazardous Substances	None of the chemicals in this product have a TPQ.
SARA Codes	CAS # 24424-99-5: flammable, reactive.
Section 313	No chemicals are reportable under Section 313.
Clean Air Act:	This material does not contain any hazardous air pollutants. This material does not contain any Class 1 Ozone depletors. This material does not contain any Class 2 Ozone depletors.
Clean Water Act:	None of the chemicals in this product are listed as Hazardous Substances under the CWA. None of the chemicals in this product are listed as Priority Pollutants under the CWA. None of the chemicals in this product are listed as Toxic Pollutants under the CWA.
OSHA:	
STATE	Di-tert-butyl dicarbonate is not present on state lists from CA, PA, MN, MA, FL, or NJ.
California Prop 65	
California No Significant Risk Level:	None of the chemicals in this product are listed.

European/International Regulations

European Labeling in Accordance with EC Directives

Hazard Symbols: T+

Risk Phrases:

R 11 Highly flammable.

R 26 Very toxic by inhalation.

R 36/37/38 Irritating to eyes, respiratory system and skin.

R 43 May cause sensitization by skin contact.

Safety Phrases:

S 7 Keep container tightly closed.

S 26 In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.

S 28 After contact with skin, wash immediately with...

S 33 Take precautionary measures against static discharges.

S 36/37/39 Wear suitable protective clothing, gloves and eye/face protection.

S 45 In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

WGK (Water Danger/Protection)

CAS# 24424-99-5: Not available

Canada

CAS# 24424-99-5 is listed on Canada's DSL List

Canadian WHMIS Classifications: B4, D1A, D2B

This product has been classified in accordance with the hazard criteria of the Controlled Products Regulations and the MSDS contains all of the information required by those regulations.

CAS# 24424-99-5 is not listed on Canada's Ingredient Disclosure List.

Section 16 - Other Information

MSDS Creation Date: 1/14/1998

Revision #8 Date 11/26/2007

Revisions were made in Sections: 2, 3, 4, 5, 6, 7, 8, 9, 10, 12

Material Safety Data Sheet

acc. to OSHA and ANSI

Printing date 11/10/2008 Reviewed on 10/01/2008

1 Identification of substance:

Product details:

Product name: Di-tert-butyl dicarbonate

Stock number:
A14708
L03289

Manufacturer/Supplier:
Alfa Aesar, A Johnson Matthey Company
Johnson Matthey Catalog Company, Inc.
30 Bond Street
Ward Hill, MA 01835-8099
Emergency Phone: (978) 521-6300
CHEMTREC: (800) 424-9300
Web Site: www.alfa.com

Information Department: Health, Safety and Environmental Department
Emergency information:
During normal hours the Health, Safety and Environmental Department.
After normal hours call Chemtrec at (800) 424-9300.

2 Composition/Data on components:

Chemical characterization:
Description: (CAS#)
Di-tert-butyl dicarbonate (CAS# 24424-99-5): 100%
Identification number(s):
EINECS Number: 246-240-1

3 Hazards identification

Hazard description:

T+ Very toxic

Information pertaining to particular dangers for man and environment
R 26 Very toxic by inhalation.
R 37/38 Irritating to respiratory system and skin.
R 41 Risk of serious damage to eyes.
R 43 May cause sensitization by skin contact.
Classification system
HMIS ratings (scale 0-4)
(Hazardous Materials Identification System)

HEALTH	3
FIRE	2
REACTIVITY	1

Health (acute effects) = 3
Flammability = 2
Reactivity = 1

4 First aid measures

General information
Immediately remove any clothing soiled by the product.
Remove breathing apparatus only after contaminated clothing has been completely removed.
In case of irregular breathing or respiratory arrest provide artificial respiration.

(Contd. on page 2)

Material Safety Data Sheet
acc. to OSHA and ANSI

Printing date 11/10/2008 Reviewed on 10/01/2008

Product name: Di-tert-butyl dicarbonate

(Contd. of page 1)

After inhalation
Supply fresh air. If required, provide artificial respiration. Keep patient warm.
Seek immediate medical advice.
After skin contact
Immediately wash with water and soap and rinse thoroughly.
Seek immediate medical advice.
After eye contact
Rinse opened eye for several minutes under running water. Then consult a doctor.
After swallowing Seek immediate medical advice.

5 Fire fighting measures

Suitable extinguishing agents
Use carbon dioxide, extinguishing powder or foam. Water may be ineffective but may be used for cooling exposed containers.
Special hazards caused by the material, its products of combustion or resulting gases:
In case of fire, the following can be released:
Carbon monoxide and carbon dioxide
Protective equipment:
Wear self-contained respirator.
Wear fully protective impervious suit.

6 Accidental release measures

Person-related safety precautions:
Wear protective equipment. Keep unprotected persons away.
Ensure adequate ventilation
Measures for environmental protection:
Do not allow material to be released to the environment without proper governmental permits.
Measures for cleaning/collecting:
Dispose contaminated material as waste according to item 13.
Ensure adequate ventilation.
Additional information:
See Section 7 for information on safe handling
See Section 8 for information on personal protection equipment.
See Section 13 for disposal information.

7 Handling and storage

Handling
Information for safe handling:
Handle under dry protective gas.
Keep container tightly sealed.
Ensure good ventilation at the workplace.
Open and handle container with care.
Only handle and refill product in closed systems.
Information about protection against explosions and fires:
Keep ignition sources away.

Storage
Requirements to be met by storerooms and receptacles: Refrigerate

(Contd. on page 3)

Material Safety Data Sheet
acc. to OSHA and ANSI

Printing date 11/10/2008 Reviewed on 10/01/2008

Product name: Di-tert-butyl dicarbonate

(Contd. of page 2)

Information about storage in one common storage facility:
Store away from oxidizing agents.
Protect from heat.
Store away from water/moisture.
Further information about storage conditions:
Store under dry inert gas.
This product is moisture sensitive.
Keep container tightly sealed.
Protect from humidity and water.
Refrigerate

8 Exposure controls and personal protection

Additional information about design of technical systems:
Properly operating chemical fume hood designed for hazardous chemicals and having an average face velocity of at least 100 feet per minute.

Components with limit values that require monitoring at the workplace:
Not required.
Additional information: No data

Personal protective equipment
General protective and hygienic measures
The usual precautionary measures for handling chemicals should be followed.
Keep away from foodstuffs, beverages and feed.
Remove all soiled and contaminated clothing immediately.
Wash hands before breaks and at the end of work.
Store protective clothing separately.
Avoid contact with the eyes and skin.
Breathing equipment:
Use suitable respirator when high concentrations are present.
Protection of hands:
Impervious gloves
Check protective gloves prior to each use for their proper condition.
Material of gloves
The selection of suitable gloves not only depends on the material, but also on quality. Quality will vary from manufacturer to manufacturer.
Eye protection: Safety glasses
Body protection: Protective work clothing.

9 Physical and chemical properties:

General Information	
Form:	Low melting solid
Color:	White
Odor:	Mild
Change in condition	
Melting point/Melting range:	22-24°C (72-75°F)
Boiling point/Boiling range:	56-57°C (133-135°F) (0.5mm Hg)
Sublimation temperature / start:	Not determined
Flash point:	84°C (183°F)

(Contd. on page 4)

Material Safety Data Sheet
acc. to OSHA and ANSI

Printing date 11/10/2008 Reviewed on 10/01/2008

Product name: Di-tert-butyl dicarbonate

(Contd. of page 3)

Ignition temperature:	460°C (860°F)
Decomposition temperature:	Not determined
Danger of explosion:	Product does not present an explosion hazard.
Explosion limits:	
Lower:	Not determined
Upper:	Not determined
Vapor pressure:	Not determined
Density at 20°C (68°F):	0.95 g/cm³
Solubility in / Miscibility with	
Water:	Slightly soluble

10 Stability and reactivity

Thermal decomposition / conditions to be avoided:
Decomposition will not occur if used and stored according to specifications.
Materials to be avoided:
Oxidizing agents
Heat
Water/moisture
Dangerous reactions No dangerous reactions known
Dangerous products of decomposition: Carbon monoxide and carbon dioxide

11 Toxicological information

Acute toxicity:

LD/LC50 values that are relevant for classification:		
Oral	LD50	>5000 mg/kg (mam)
		>5000 mg/kg (rat)
Dermal	LD50	>2000 mg/kg (mam)
		>2000 mg/kg (rabbit)
Inhalative	LC50/4H	100 mg/m3/4H (rat)

Primary irritant effect:
on the skin: Irritant to skin and mucous membranes.
on the eye: Strong irritant with the danger of severe eye injury.
Sensitization: Sensitization possible through skin contact.
Subacute to chronic toxicity:
Extrnal MSDS reports that exposure to mist or aerosol may cause irreversible ocular opacity.
Subacute to chronic toxicity:
The Registry of Toxic Effects of Chemical Substances (RTECS) reports the following effects in laboratory animals:
Sense Organs and Special Senses (Eye) - effect, not otherwise specified.
Lungs, Thorax, or Respiration - dyspnea.
Nutritional and Gross Metabolic - weight loss or decreased weight gain.

(Contd. on page 5)

Material Safety Data Sheet
acc. to OSHA and ANSI

Printing date 11/10/2008 Reviewed on 10/01/2008

Product name: Di-tert-butyl dicarbonate

(Contd. of page 4)

Additional toxicological information:
To the best of our knowledge the acute and chronic toxicity of this substance is not fully known.
No classification data on carcinogenic properties of this material is available from the EPA, IARC, NTP, OSHA or ACGIH.

12 Ecological information:

General notes:
Do not allow undiluted product or large quantities of it to reach ground water, water course or sewage system.
Do not allow material to be released to the environment without proper governmental permits.

13 Disposal considerations

Product:
Recommendation
Consult state, local or national regulations to ensure proper disposal.

Uncleaned packagings:
Recommendation: Disposal must be made according to official regulations.

14 Transport information

DOT regulations:

Hazard class:	6.1
Identification number:	UN2811
Packing group:	II
Proper shipping name (technical name):	TOXIC SOLID, ORGANIC, N.O.S. (Di-tert-butyl dicarbonate)
Label	6.1

Land transport ADR/RID (cross-border)

ADR/RID class:	6.1 (T2) Toxic substances
Danger code (Kemler):	60
UN-Number:	2811
Packaging group:	II

(Contd. on page 6)

Material Safety Data Sheet
acc. to OSHA and ANSI

Printing date 11/10/2008 Reviewed on 10/01/2008

Product name: Di-tert-butyl dicarbonate

(Contd. of page 5)

Description of goods:	2811 TOXIC SOLID, ORGANIC, N.O.S. (Di-tert-butyl dicarbonate)

Maritime transport IMDG:

IMDG Class:	6.1
UN Number:	2811
Label	6.1
Packaging group:	II
Proper shipping name:	TOXIC SOLID, ORGANIC, N.O.S. (Di-tert-butyl dicarbonate)

Air transport ICAO-TI and IATA-DGR:

ICAO/IATA Class:	6.1
UN/ID Number:	2811
Label	6.1
Packaging group:	II
Proper shipping name:	TOXIC SOLID, ORGANIC, N.O.S. (Di-tert-butyl dicarbonate)

15 Regulations

Product related hazard informations:

Hazard symbols:
T+ Very toxic

Risk phrases:
26 Very toxic by inhalation.
37/38 Irritating to respiratory system and skin.
41 Risk of serious damage to eyes.
43 May cause sensitization by skin contact.

Safety phrases:
26 In case of contact with eyes, rinse immediately with plenty of water and seek medical advice.
28 After contact with skin, wash immediately with plenty of water
36/37/39 Wear suitable protective clothing, gloves and eye/face protection.
45 In case of accident or if you feel unwell, seek medical advice immediately.

National regulations
All components of this product are listed in the U.S. Environmental Protection Agency Toxic Substances Control Act Chemical substance Inventory.
All components of this product are listed on the Canadian Domestic Substances List (DSL).

(Contd. on page 7)

Material Safety Data Sheet
acc. to OSHA and ANSI

Printing date 11/10/2008 *Reviewed on 10/01/2008*

Product name: Di-tert-butyl dicarbonate

(Contd. of page 6)

Information about limitation of use:
For use only by technically qualified individuals.

16 Other information:
Employers should use this information only as a supplement to other information gathered by them, and should make independent judgement of suitability of this information to ensure proper use and protect the health and safety of employees. This information is furnished without warranty, and any use of the product not in conformance with this Material Safety Data Sheet, or in combination with any other product or process, is the responsibility of the user.

Department issuing MSDS: *Health, Safety and Environmental Department.*
Contact: *Paul V. Connolly*

SAFETY DATA SHEET

DI-TERT-BUTYLDICARBONATE

1. IDENTIFICATION OF THE SUBSTANCE/PREPARATION AND COMPANY/UNDERTAKING

Synonyms	Diboc
Chemical characterization	Solid. Liquid.
Product code	1001021, 1011664, 3515019
Supplier	Siber Hegner Raw Materials LTD. P.O.Box 888 CH-8034 Zürich Switzerland 01 386 73 46
Emergency telephone number	++41 1 386 73 46

2. COMPOSITION/INFORMATION ON INGREDIENTS

Hazardous components	CAS No. : 24424-99-5 EINECS No. : 256-240-1

3. HAZARDS IDENTIFICATION

Irritating to eyes and skin. May cause s
contact. Flammable. Harmful in contact
swallowed. Very toxic by inhalation.

4. FIRST AID MEASURES

Inhalation	Move to fresh air. Oxygen or artificial re Consult a physician for severe cases.
Skin contact	Wash off immediately with soap and pla
Eye contact	Rinse immediately with plenty of water, eyelids, for at least 15 minutes. If eye ir consult a specialist.
Ingestion	Rinse mouth.

5. FIRE-FIGHTING MEASURES

Suitable extinguishing media Carbon dioxide (CO2). Foam. Dry powder.

Special protective equipment for firefighters
Wear protective suit. Wear self contained breathing apparatus for fire fighting if necessary.

6. ACCIDENTAL RELEASE MEASURES

Personal precautions Do not breathe gas/fumes/vapour/spray.

Environmental precautions Do not flush into surface water or sanitary sewer system.

Methods for cleaning up Sweep up and shovel. Soak up with inert absorbent material (e.g. sand, silica gel, acid binder, universal binder, sawdust).

7. HANDLING AND STORAGE

Handling Avoid contact with skin and eyes. Keep away from sources of ignition - No smoking.

Storage Keep containers tightly closed in a dry, cool and well-ventilated place. Keep at temperatures below 10 °C.

8. EXPOSURE CONTROLS / PERSONAL PROTECTION

Personal protection equipment

Respiratory protection In case of insufficient ventilation wear suitable respiratory equipment.

Hand protection Protective gloves.

Eye protection Safety glasses.

Skin and body protection Protective suit.

9. PHYSICAL AND CHEMICAL PROPERTIES

Form Solid. Liquid.

Colour White. Colourless.

Physical and chemical properties
Melting point/range 22 - 24°C.
Boiling point/range 56 - 57°C. (0.5 mmHg).
Density 1.02 g/cm3 (20°C).
Water solubility: insoluble.
Flash point 73 - 83°C.
Autoignition temperature 460°C.
Formula: C10H18O5.

10. STABILITY AND REACTIVITY

Stability	Stable under recommended storage conditions.
Conditions to avoid	Product is sensitive to light and moisture. Heating in air.
Materials to avoid	Incompatible with strong acids and oxidizing agents. Reducing agents.
Hazardous decomposition products	Carbon monoxide. Carbon oxides.

11. TOXICOLOGICAL INFORMATION

Acute toxicity	LD50/oral/rat = > 5000 mg/kg. LD50/dermal/rabbit = > 2000 mg/kg. LC50/inhalation/4h/rat = 0.10 mg/l.

12. ECOLOGICAL INFORMATION

Ecotoxicity	No data available.

13. DISPOSAL CONSIDERATIONS

Waste from residues / unused products	Can be landfilled or incinerated, when in compliance with local regulations.

14. TRANSPORT INFORMATION

Proper shipping name	Flammable solid, organic, n.o.s.*
UN-No	1325
ADR/RID	Class 4.1. Item 6c. ADR/RID-Labels 4.1. TREM-CARD 41G01. Kemler code 46.
IMO	Class 4.1. Packaging group III. IMDG Page 4146. EmS 4.1-05.
ICAO	Class 4.1. Packaging group III. Packing instruction (passenger aircraft): 419. Maximum quantity 25 kg. Packing instruction (cargo aircraft): 420. Maximum quantity 100 kg.

15. REGULATORY INFORMATION

Symbol(s)	Xn - Harmful.
R-phrase(s)	R10: Flammable. R21/22: Harmful in contact with skin and if swallowed. R26: Very toxic by inhalation. R36/37/38: Irritating to eyes, respiratory system and skin. R43: May cause sensitization by skin contact.
S-phrase(s)	S23: Do not breathe vapour. S24/25: Avoid contact with skin and eyes.

16. OTHER INFORMATION

Disclaimer	The data and information given on the safety data sheet are based on literature and/or documentation submitted to us. These data do not guarantee any properties and do not dispense with the need for tests and investigations being made by the end-user. Existing regulations and laws have to be observed by the customer on his own responsability.
Revision Date	2/12/97, 2/6/98
Number	1

MATERIAL SAFETY DATA SHEET

Date Printed: 05/01/2009
Date Updated: 06/06/2008
Version 1.10

Section 1 - Product and Company Information

Product Name	DI-TERT-BUTYL DICARBONATE, REAGENTPLUS, >=99%
Product Number	361941
Brand	ALDRICH
Company	Sigma-Aldrich
Address	3050 Spruce Street SAINT LOUIS MO 63103 US
Technical Phone:	800-325-5832
Fax:	800-325-5052
Emergency Phone:	314-776-6555

Section 2 - Composition/Information on Ingredient

Substance Name	CAS #	SARA 313
DI-TERT-BUTYL DICARBONATE	24424-99-5	No

Formula	C10H18O5
Synonyms	Bis(1,1-dimethylethyl) dicarbonate * BOC-anhydride * tert-Butyl dicarbonate * Di-tert-butyl oxydiformate * Di-tert-butyl pyrocarbonate * Formic acid, oxydi-, di-tert-butyl ester (7CI,8CI * Pyrocarbonic acid di-tert-butyl ester
RTECS Number:	HT0230000

Section 3 - Hazards Identification

EMERGENCY OVERVIEW

Flammable. Highly Toxic (USA) Very Toxic (EU).
Very toxic by inhalation. Irritating to eyes, respiratory system and skin.
May develop pressure.

HMIS RATING

HEALTH: 3
FLAMMABILITY: 3
REACTIVITY: 0

NFPA RATING

HEALTH: 3
FLAMMABILITY: 3
REACTIVITY: 0

For additional information on toxicity, please refer to Section 11.

Section 4 - First Aid Measures

ORAL EXPOSURE

If swallowed, wash out mouth with water provided person is conscious. Call a physician immediately.

INHALATION EXPOSURE
If inhaled, remove to fresh air. If not breathing give artificial respiration. If breathing is difficult, give oxygen.

DERMAL EXPOSURE
In case of skin contact, flush with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes. Call a physician.

EYE EXPOSURE
In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Call a physician.

Section 5 - Fire Fighting Measures

FLAMMABLE HAZARDS
Flammable Hazards: Yes

EXPLOSION HAZARDS
Vapor may travel considerable distance to source of ignition and flash back. Container explosion may occur under fire conditions. Forms explosive mixtures in air.

FLASH POINT
98.6 °F 37 °C Method: closed cup

AUTOIGNITION TEMP
N/A

FLAMMABILITY
N/A

EXTINGUISHING MEDIA
Suitable: For small (incipient) fires, use media such as "alcohol" foam, dry chemical, or carbon dioxide. For large fires, apply water from as far as possible. Use very large quantities (flooding) of water applied as a mist or spray; solid streams of water may be ineffective. Cool all affected containers with flooding quantities of water.

FIREFIGHTING
Protective Equipment: Wear self-contained breathing apparatus and protective clothing to prevent contact with skin and eyes.
Specific Hazard(s): Flammable liquid. Emits toxic fumes under fire conditions.
Specific Method(s) of Fire Fighting: Use water spray to cool fire-exposed containers.

Section 6 - Accidental Release Measures

PROCEDURE TO BE FOLLOWED IN CASE OF LEAK OR SPILL
Evacuate area. Shut off all sources of ignition. Use nonsparking tools.

PROCEDURE(S) OF PERSONAL PRECAUTION(S)
Wear self-contained breathing apparatus, rubber boots, and heavy rubber gloves.

METHODS FOR CLEANING UP
Cover with dry-lime, sand, or soda ash. Place in covered

containers using non-sparking tools and transport outdoors. Ventilate area and wash spill site after material pickup is complete.

Section 7 - Handling and Storage

HANDLING

User Exposure: Always open containers slowly to allow any excess pressure to vent. Do not breathe vapor. Do not get in eyes, on skin, on clothing. Avoid prolonged or repeated exposure.

STORAGE

Suitable: Keep tightly closed. Keep away from heat, sparks, and open flame.
Incompatible Materials: Avoid contact with acid.
Store at 2-8°C

SPECIAL REQUIREMENTS

May develop pressure. Open carefully.

Section 8 - Exposure Controls / PPE

ENGINEERING CONTROLS

Safety shower and eye bath. Use nonsparking tools. Use only in a chemical fume hood.

PERSONAL PROTECTIVE EQUIPMENT

Respiratory: Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU). Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator.
Hand: Compatible chemical-resistant gloves.
Eye: Chemical safety goggles.

GENERAL HYGIENE MEASURES

Wash contaminated clothing before reuse. Wash thoroughly after handling.

Section 9 - Physical/Chemical Properties

Appearance	Physical State: Clear liquid Color: Colorless	
Property	Value	At Temperature or Pressure
Molecular Weight	218.25 AMU	
pH	N/A	
BP/BP Range	56.0 - 57.0 °C	0.5 mmHg
MP/MP Range	22 °C	
Freezing Point	N/A	
Vapor Pressure	N/A	
Vapor Density	N/A	
Saturated Vapor Conc.	N/A	
SG/Density	0.95 g/cm3	
Bulk Density	N/A	
Odor Threshold	N/A	
Volatile%	N/A	
VOC Content	N/A	
Water Content	N/A	

Solvent Content	N/A	
Evaporation Rate	N/A	
Viscosity	N/A	
Surface Tension	N/A	
Partition Coefficient	N/A	
Decomposition Temp.	N/A	
Flash Point	98.6 °F 37 °C	Method: closed cup
Explosion Limits	N/A	
Flammability	N/A	
Autoignition Temp	N/A	
Refractive Index	1.409	
Optical Rotation	N/A	
Miscellaneous Data	N/A	
Solubility	N/A	

N/A = not available

Section 10 - Stability and Reactivity

STABILITY

Stable: Stable.
Materials to Avoid: Oxidizing agents, Reducing agents Avoid contact with acid., Bases

HAZARDOUS DECOMPOSITION PRODUCTS

Hazardous Decomposition Products: Carbon monoxide, Carbon dioxide.

HAZARDOUS POLYMERIZATION

Hazardous Polymerization: Will not occur

Section 11 - Toxicological Information

ROUTE OF EXPOSURE

Skin Contact: Causes skin irritation.
Skin Absorption: May be harmful if absorbed through the skin.
Eye Contact: Causes eye irritation.
Inhalation: Highly toxic by inhalation. Material is irritating to mucous membranes and upper respiratory tract.
Ingestion: May be harmful if swallowed.

TOXICITY DATA

Inhalation
Rat
100 mg/m3
LC50
Remarks: Nutritional and Gross Metabolic:Weight loss or decreased weight gain. Lungs, Thorax, or Respiration:Dyspnea. Sense Organs and Special Senses (Nose, Eye, Ear, and Taste):Eye:Other.

Oral
Mammal
> 5000 mg/kg
LD50

Skin
Mammal
> 2000 mg/kg
LD50

Section 12 - Ecological Information

No data available.

Section 13 - Disposal Considerations

APPROPRIATE METHOD OF DISPOSAL OF SUBSTANCE OR PREPARATION
Contact a licensed professional waste disposal service to dispose of this material. Dissolve or mix the material with a combustible solvent and burn in a chemical incinerator equipped with an afterburner and scrubber. Observe all federal, state, and local environmental regulations.

Section 14 - Transport Information

DOT
Proper Shipping Name: Toxic liquids, flammable, organic, n.o.s.
UN#: 2929
Class: 6.1
Packing Group: Packing Group I
Hazard Label: Toxic substances.
Hazard Label: Flammable liquid
PIH: Not PIH

IATA
Proper Shipping Name: Toxic liquid, flammable, organic, n.o.s.
IATA UN Number: 2929
Hazard Class: 6.1
Packing Group: I
Not Allowed - Aircraft: Cargo aircraft only. Not permitted on passenger aircraft.

Section 15 - Regulatory Information

EU ADDITIONAL CLASSIFICATION
Symbol of Danger: T+
Indication of Danger: Very toxic.
R: 10-26-36/37/38
Risk Statements: Flammable. Very toxic by inhalation. Irritating to eyes, respiratory system and skin.
S: 7/9-16-26-28-36/37-45
Safety Statements: Keep container tightly closed and in well-ventilated place. Keep away from sources of ignition - no smoking. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. After contact with skin, wash immediately with plenty of water. Wear suitable protective clothing and gloves. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

US CLASSIFICATION AND LABEL TEXT
Indication of Danger: Flammable. Highly Toxic (USA) Very Toxic (EU).
Risk Statements: Very toxic by inhalation. Irritating to eyes, respiratory system and skin.
Safety Statements: Keep away from sources of ignition - no smoking. In case of contact with eyes, rinse immediately with plenty of water and seek medical advice. Wear suitable protective clothing and gloves. In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

US Statements: May develop pressure.

UNITED STATES REGULATORY INFORMATION
SARA LISTED: No

CANADA REGULATORY INFORMATION
WHMIS Classification: This product has been classified in accordance with the hazard criteria of the CPR, and the MSDS contains all the information required by the CPR.
DSL: Yes
NDSL: No

Section 16 - Other Information

DISCLAIMER
For R&D use only. Not for drug, household or other uses.

WARRANTY
The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Inc., shall not be held liable for any damage resulting from handling or from contact with the above product. See reverse side of invoice or packing slip for additional terms and conditions of sale.