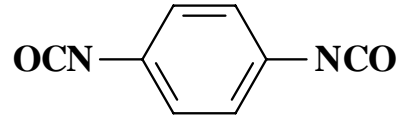




DuPont Chemical Solutions Enterprise

Technical Information



Para-Phenylenediisocyanate (PPDI)

Product Description

DuPont PPDI is a specialty isocyanate which can provide cast and thermoplastic elastomers with properties unmatched by other commercial polyurethanes. Due to its small size and symmetry, the PPDI molecule provides a compact hard segment and excellent phase separation in polyurethane formulations. DuPont PPDI-based elastomers show:

- Superior dynamic properties
- Exceptional abrasion resistance and flex fatigue
- Low compression set at elevated temperatures
- High temperature performance to 135C (275F) in continuous use

DuPont PPDI is available as a free-flowing solid.

Uses

DuPont PPDI is especially suitable for applications in these demanding environments:

- Hot moist environments
- Oily environments
- Tear- and abrasion-prone applications
- Power-driven, repeat motion applications

Products using PPDI include seals and gaskets, pump diaphragms and oilfield service materials as well as power couplings, belts, jounce bumpers, shock absorbers, rollers and load-bearing wheels. PPDI-based elastomers serve markets in power tools, mining, automotive, sporting goods and office equipment.

Product Specifications

<u>Property, units</u>	<u>Specification</u>
Purity, wt. %	98.5 min
Residual solvent, ppm	500 max.
Hydrolyzable chlorides, ppm	200 max

Hazards

Like most isocyanates, PPDI is reactive and toxic, and must be handled only by trained personnel. All exposure should be avoided. See the PPDI MSDS for additional handling information.

To enjoy the performance advantages of PPDI without handling the isocyanate directly, contact us regarding low toxicity prepolymers and thermoplastic elastomers based on PPDI.

Packages and Shipping Information

DuPont PPDI is available in three package sizes, described below.

DOT Shipping name	Toxic Solid, NOS (para-phenylene diisocyanate)
DOT Hazard Classification	Poison
UN/NA No.	UN 2811
Packing Group	II
Packages	90.7 kg (200 lb) and 10 kg (22 lb) net drums 0.5 kg (1 lb) net sample

Physical Properties

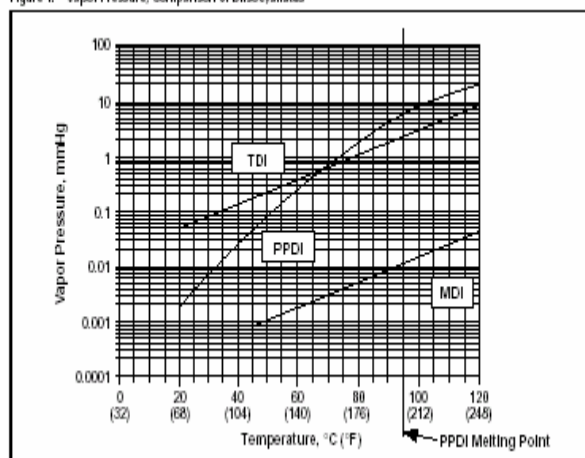
Table 1 shows typical physical properties for DuPont PPDI. The vapor pressure of PPDI is near that of TDI (toluene diisocyanate), which is widely used in the industry. Figure 1 illustrates the comparison of vapor pressures of PPDI to common diisocyanates, over the range of normal handling and processing temperatures. Note that at room temperatures, PPDI has a slightly lower vapor pressure than TDI. Nevertheless, it is high enough to exceed the upper exposure limit (STEL) at room temperature, and thus care must be taken to avoid personnel exposure during handling and processing. PPDI also has a tendency to sublime; see further discussion in section on processing.

Table 1

Typical Physical Properties of DuPont PPDI	
Formula	$C_6H_4(NCO)_2$
CAS Registry No.	104-49-4
Molecular Weight	160.1
NCO Content, %	52.5
Isocyanate Equivalent Weight	80.0
Melting Point, °C (°F)	94 (201)
Boiling Point, 760 mmHg, °C (°F)	260 (500)
Vapor Pressure at 20°C, mmHg	0.002
at 95°C, mmHg	5.07
Specific Gravity at 100°C	1.17
Flash Point, CCCM, °C (°F)	120 (248)
Viscosity at 100°C, cP	1.13
Heat of Fusion, J/kg	184
cal/g	44
Specific Heat	0.3
Approximate Bulk Density of Flake	40 lb/ft ³ (641 kg/m ³)

Figure 1. Vapor Pressure Comparison of Diisocyanates

Figure 1. Vapor Pressure, Comparison of Diisocyanates



Chemical Properties

Table 2 gives solubilities of PPDI in common organic solvents. PPDI behaves chemically as a typical reactive aromatic diisocyanate such as TDI or MDI. It reacts exothermally with alcohols, amines, and other compounds containing active hydrogen. PPDI is incompatible with strong acids, strong alkalis, strong oxidizers, and water.

Table 2

Solubility of DuPont PPDI in Various Solvents

Solvent	g/100 g solvent	
	23°C (73°F)	40°C (104°F)
Toluene	13	23
Acetone	18	25
Ethyl Acetate	16	28
Cellosolve Acetate	13	16
Tetrahydrofuran	25	28
Perchloroethylene	7	14

Using DuPont PPDI in Prepolymers and Cast Elastomers

Prepolymer Procedure

1. Drying and Degassing Polyol

To remove dissolved gases and traces of water, stir the polyol at 90–100°C (194–212°F) while alternately sparging with dry nitrogen and applying full oil-pump vacuum.

2. Prepolymer Reaction

Add flaked PPDI all at once to polyol at 70–80°C (158–176°F) under pad of dry nitrogen with good agitation. The PPDI will dissolve within 45 minutes. The reaction must be cooled to maintain a reaction temperature of 80–90°C (176–194°F) and should be complete in about two hours.

PPDI can sublime to cooler surfaces of the reaction vessel, causing a change in reaction stoichiometry and plugging lines. Minimize cooler exposed surfaces by operating with full reactor and heated surfaces.

Verify completeness of reaction by observing approach of percent NCO values to theoretical. Determine the viscosity. The viscosity of a 2-to-1 prepolymer made with Terathane® 2000 polyol should be about 12,000–14,000 cP at 30°C (86°F).

For use within several days, the prepolymer may be maintained in its molten state at 60°C (140°F) under dry nitrogen. The prepolymer is stable if stored under dry nitrogen in sealed drums at room temperature.

Casting Procedure

1. Curing and Molding

Mix ratios of 25:1 may be required, so a high quality machine for metering, mixing, and dispensing is essential for best results. Preheat the prepolymer to 80°C (176°F) and degas. The curative may be used at room temperature, but should be dry and degassed. After mixing, “open times” of 3–4 minutes are usually observed. Mold temperatures close to 150°C (302°F) should be used. The minimum mold temperature is 120°C (248°F).

Parts can usually be demolded after 30 minutes.

1,4-butanediol is an excellent curative for prepolymers of PPDI. Special blends of curatives may be used to achieve various hardnesses and other desired properties. An NCO/OH cure ratio of 1.075 is recommended as a starting point for optimization. If this ratio drops close to or below 1.0, significant property loss may result.

2. Postcuring

Postcure at 100–120°C (212–248°F) for at least 16 hours in a ventilated oven under nitrogen sweep. Allow approximately three weeks at ambient conditions for development of full physical properties.

Personal Safety and Handling

Refer to the MSDS before handling PPDI. Avoid personal exposure to PPDI. Contact with PPDI may cause eye burns, and irritation to lungs, skin and other body surfaces. As with other isocyanates, PPDI may also cause respiratory sensitization producing asthma-like symptoms after repeated exposures.

The DuPont Acceptable Exposure Limit (AEL) for PPDI is 0.03 mg/m³ as aerosol/vapor, and 0.005 ppm as vapor/vapor, 8- and 12-hour Time Weighted Average (TWA) for particulate and vapor (combined). This limit is similar to that for TDI.

Personal Protective Equipment

Employees should use chemical splash goggles and face shield to prevent eye contact. Use a NIOSH/MSHA-approved air-supplied respirator with full-face mask if concentrations in the work area exceed exposure limits. Wear gloves, apron, boots, or whole body suits as appropriate to avoid contact. Disposable clothing such as Tyvek® coveralls is recommended when handling solid PPDI for short periods of time.

Air Monitoring

Monitoring for personnel exposure is necessary when working with PPDI. Personnel badges that have been calibrated for PPDI are available from Scott/Bacharach, 251 Welsh Pool Rd, Exton, Pa 19341, phone 610-363-5450. Stationary PPDI monitors can be ordered from Zellweger Analytics, 405 Barclay Blvd., Lincolnshire, IL 60069, phone 847-955-8200.

Medical Surveillance

Establish a medical evaluation and surveillance program to cover new and existing employees. Any employee who has been diagnosed as being sensitized to diisocyanates must be removed from any subsequent diisocyanate exposure.

Product Storage

DuPont PPDI may be stored indefinitely at temperatures below 40°C (104°F). Dimerization will occur in the solid phase as well as in the liquid phase at higher temperatures near the melting point, but dimerization is not an issue in normal storage and use. Detailed kinetic data may be obtained upon request.

Store PPDI in a well-ventilated area. Do not open the drums until ready to use. If the contents of a drum are only partially consumed, the drum should be purged with dry nitrogen and tightly resealed. Reaction with water vapor in the air will cause degradation of the product into carbon dioxide and a “urea compound.” An indication that this may have happened is when the flakes do not subsequently dissolve or react rapidly in a diol reaction mixture. This is caused by a thin surface coating of the “urea compound,” which protects the remaining PPDI from further reaction. Avoid exposure of PPDI to moisture.

Processing Considerations

PPDI should be handled in a chemical hood or in an area with adequate local ventilation. Vents from process equipment should be scrubbed with appropriate solvent prior to discharge to atmosphere. PPDI sublimate will condense on cooler surfaces; therefore, all vent piping must be heat traced and insulated upstream of the scrubbing equipment. Care should be taken to ensure that condensate and sublimate do not interfere with proper operation of safety devices such as relief valves and rupture disks.

Materials of Construction

Stainless steel construction is recommended for all process equipment handling PPDI. Storage containers should be stainless steel or coated with a baked phenolic resin. Avoid contact with metals such as zinc, copper, tin, and cadmium.

Spill Cleanup

Spill cleanup and waste disposal procedures are similar to those for other isocyanates, except a unique characteristic must be considered and addressed. In contrast to some other isocyanates, only fine particles of PPDI can be readily deactivated with water or ammonia/water systems. In the case of larger particles or lumps, a “crust” or “skin” of “urea compound” forms on the outer surface, leaving an inner “core” of PPDI. Any deactivation procedure must provide breakup into smaller particles or exposure to deactivation agent for extended periods of time.

Spills of PPDI should be handled as follows:

- Evacuate and barricade the area.
- Employees entering a barricaded spill area must wear proper protective equipment, including a full-face air-supplied respirator.
- Decontaminate the spill and surrounding floor area with a deactivating agent, such as one of the following:
 - 8% concentrated ammonia solution, 2% detergent, and balance water
 - Hot water or steam
 - 50/50 mixture of isopropyl alcohol and triethanol amine
- Monitor the spill area for active PPDI with portable monitor or personnel badges.
- Place the spill cleanup material in an appropriate container, and dispose of solids as outlined in the Waste Disposal section of this bulletin.

For PPDI solutions that remain a liquid at room temperature, add the following steps to the procedure for handling solid PPDI spills:

- Dike the spill area with an absorbent material (sand, absorbent clay, etc.).
- Cover the spill with an absorbent/neutralizing mixture such as:
 - 60 wt% absorbent material (sawdust, fuller’s earth, etc.)
 - 40 wt% ammonia aqueous solution
- Shovel contaminated absorbent into open-top steel drums and store in a ventilated area with lids loosely sealed for several days to allow any residual carbon dioxide gas to escape. Once the drums are sealed tightly, follow the procedures under Waste Disposal.

Waste Disposal

Waste PPDI should be neutralized prior to disposal. The exact method used depends on quantities of waste on hand.

- The preferred method is to react the PPDI with excess polyol to make a low-quality polymer or foam that can be incinerated or landfilled. The PPDI must dissolve in the polyol in order to fully react. Heating is typically required to complete the reaction.
- DuPont PPDI can be incinerated, but this should be done *only* in properly supervised equipment specifically designed and licensed for the disposal of noxious chemical wastes.

Treatment, storage, transportation, and disposal must always be done in accordance with federal, state, and local regulations.

Drum Disposal

Empty drums will contain residual traces of PPDI. Drums should be decontaminated before disposal as follows:

1. Remove all solid particles.
2. Rinse with a deactivating solution such as: 8% concentrated ammonia solution, 2% detergent, and balance water.
3. Repeat the rinse, and then fill the drum with the deactivating solution a third time. Drums should *not* be sealed tightly and should be allowed to stand for 24 hours to allow all of the isocyanate to react. Drums should then be emptied and rinsed with water. Drums should be punctured, crushed, and disposed of in an approved landfill.

Order Placement and Product Information

Please contact us to place an order, request a sample, or obtain additional information on DuPont PPDI and related products. DuPont is available worldwide to serve your needs:

United States

Phone (800) 441-9508 (within the US)
302-892-8254 (outside the US)
Fax 302-892-1456
Mail DuPont Chemical Solutions Enterprise
Customer Service Center, BMP 23
Wilmington, DE 19899 USA

DuPont Subsidiaries - Contact the office nearest you:

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Asia Pacific	
DuPont Kabushiki Kaisha	81 3 5521 8670
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DuPont (Korea) Inc	82 2 2222 5309
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DuPont Co (Singapore) Pte Ltd	65 6586 3626
DuPont Australia Ltd	61 2 9923 6111
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DuPont de Nemours (UK) DCSE@lux.dupont.com	+44 1422 218 545
North/South America	
DuPont Canada, Inc	905 821 5912
DuPont do Brasil	55 11 4166-8337

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