

## Durasyn<sup>®</sup> Polyalphaolefins: Summary of Environmental Data

The environmental data on polyalphaolefins (PAOs) were obtained from a variety of sources, using PAOs from different producers. Durasyn<sup>®</sup> polyalphaolefins<sup>1</sup> were used only in those tests so designated.

Ecotoxicity data of neat materials is useful in choosing between components for a formulation. Because additives can greatly affect a product's environmental properties, it is important to test a fully formulated product in order to best assess its true environmental impact.

- Polyalphaolefins are considered non-toxic and non-irritating to mammals.
- Durasyn<sup>®</sup> polyalphaolefins are not expected to be toxic to aquatic organisms.
- The lower viscosity Durasyn<sup>®</sup> Polyalphaolefins (2, 4 cSt) are easily biodegraded in aquatic environments under CEC L33 A-94 test procedure conditions.
- The higher viscosity Durasyn<sup>®</sup> Polyalphaolefins (6 cSt and above) are not significantly biodegraded in the time span of the standard CEC L33 A-94 method.
- In a time-extended CEC L33 A-94 experiment, 2, 4, and 8 cSt Durasyn<sup>®</sup> Polyalphaolefins continue to biodegrade well past the 21 days prescribed in the standard method.
- Durasyn<sup>®</sup> Polyalphaolefins are not bioresistant.
- Polyalphaolefins are not expected to bioaccumulate in aquatic organisms.

<sup>1</sup> Durasyn is a registered trademark of INEOS Oligomers a division of INEOS USA LLC.

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## TOXICITY

### Mammalian Toxicity

**Polyalphaolefins are considered non-toxic and non-irritating to mammals.**

They are expected to be:

- Not acutely toxic if exposure occurs by oral routes <sup>(A)</sup>
- Non-hazardous by inhalation under conditions of normal use <sup>(B)</sup>
- Non-irritating to eyes <sup>(C)</sup>
- Non-comedogenic <sup>(D)</sup>
- Non-irritating to skin <sup>(C)</sup>
- Non-sensitizing to skin <sup>2(C)</sup>

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Table 1

Polyalphaolefins Acute Mammal Toxicity				
PAO	(A) Oral LD <sub>50</sub>	(C) Skin Irritation	(E) Eye Irritation <sup>3</sup>	(D) Comedo- genicity <sup>3</sup>
2 cSt	>5 g/kg	negative	negative	negative
4 cSt	>5 g/kg	negative	negative	negative
6 cSt	>5 g/kg	negative	negative	negative
8 cSt	>5 g/kg	negative	negative	negative
10 cSt	>5 g/kg	negative	negative	negative

(A) Rat oral LD<sub>50</sub> (statistically calculated dose needed to kill 50% of the rats in the study) is determined by single-dose administration of undiluted test material. Rat oral LD<sub>50</sub> values of >5 g/kg are considered non-toxic.

(B) Where heated material or oil mists could be generated, consult the MSDS for recommended handling procedures.

(C) According to criteria of Federal Hazardous Substance and Articles regulations (16CFR 1500).

(D) Comedogenicity refers to the ability of the test material to induce the enhanced collection of increased sebaceous material and keratin likened to acne blemishes.

<sup>2</sup>"Toxicity of Lubricating Oils," Warne, T.M., and Halder, C.A., Presented at the 40th Annual Meeting, American Society of Lubrication Engineers, 1985.

<sup>3</sup> These studies were conducted for Quantum Chemical Corporation, Emery Division, by independent contract-laboratories in 1988 and 1989. The Quantum PAO plant is now owned and operated by INEOS Oligomers

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## Aquatic Toxicity

**Durasyn<sup>®</sup> Polyalphaolefins are not expected to be toxic to aquatic organisms.**

In a Microtox<sup>4</sup> test, the Durasyn<sup>®</sup> Polyalphaolefins had no toxic effects for concentrations up to 49,500 ppm of the Water Soluble Fraction (WSF).

In general, PAOs are not readily bioavailable to aquatic organisms. This is due primarily to their low water solubility. Thus, PAOs are anticipated to be relatively inert in aquatic systems. (Please refer to the section on “Bioaccumulation.”)

Table 2

Aquatic Toxicity via the Microtox Method*	
Durasyn PAO	EC <sub>50</sub>
162	NR
164	NR
166	NR
168	NR
170	NR
174I&R	NR
180I&R	NR

\* — WSF tested

NR — No toxic response at concentrations up to 49,500 ppm

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## The Microtox Test

The Microtox test is a method for quantifying aquatic toxicity. In this experiment, bioluminescent marine bacteria are exposed for short periods (minutes) to test substances. Any changes in the microorganisms' metabolic processes will cause changes in their light output. Reduction in their light output is proportional to the toxicity of the sample. Toxicity is quantified in terms of an "EC50," the "effective concentration" at which the light emissions decrease by 50%.

The Water Soluble Fractions (WSF) were prepared by extracting the PAOs with synthetic seawater. The aqueous extracts were then evaluated in the Microtox test. This procedure is commonly used to assay water-insoluble materials.

## BIODEGRADABILITY

The lower viscosity Durasyn<sup>®</sup> Polyalphaolefins (2 and 4 cSt) are easily biodegraded in aquatic environments.

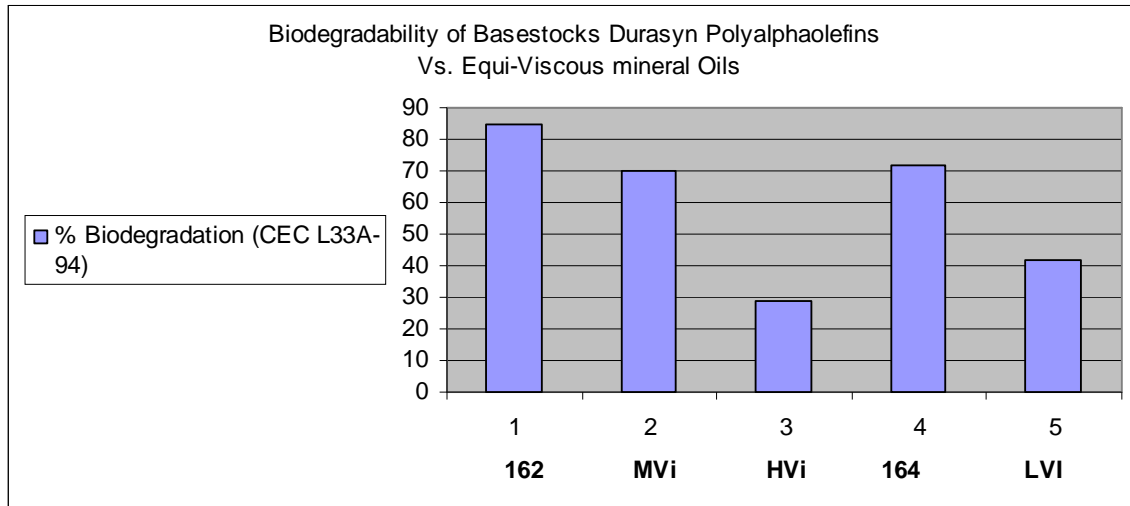
Graph 1 shows that Durasyn 162 and 164 Polyalphaolefins are significantly biodegraded in the CEC L33 A-94 experiment. This graph also shows the biodegradability of some equi-viscous naphthenic and paraffinic mineral oil basestocks. The low- viscosity Durasyn<sup>®</sup> Polyalphaolefins clearly outperform these other basestocks in this biodegradability assay.

<sup>4</sup> Microtox is a registered trademark of Azur Environmental, Carlsbad, CA, (<http://www.azurenv.demon.co.uk/>).

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Graph 1



#### Basestock

**MVi** - Medium Viscosity Index (Naphthenic Basestock;

Aromatic Content 1.9%)

**HVi** - High Viscosity Index (Paraffinic Basestock;

Aromatic Content 2.6%)

**LVi** - Low Viscosity Index (Naphthenic Basestock;

Aromatic Content 12.3%)

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**The higher viscosity Durasyn<sup>®</sup> Polyalphaolefins (6cSt and above) are not significantly biodegraded in the time span of the standard CEC L33 A-94 method.**

One can speculate that the slow rates of biodegradation found with higher viscosity PAOs are attributable to their:

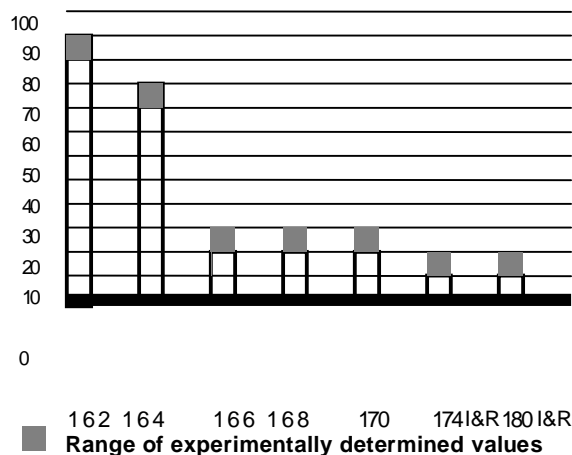
- high degree of branching
- extremely low water solubility and thus low bioavailability

A range of biodegradability values, experimentally measured, are reported in Graph 2 for each of the viscosity grades. These PAO fluids were tested repeatedly at different laboratories at different times of the year. This range of biodegradability values is quite expected, considering the variability of the source of the inoculum. (See below for a more detailed description of the CEC L33 A-94 test.)

These results with the higher viscosity PAOs may explain the overly generalized, inaccurate perception that all PAOs are not biodegradable.

Graph 2

## Biodegradability of Durasyn<sup>®</sup> Polyalphaolefins



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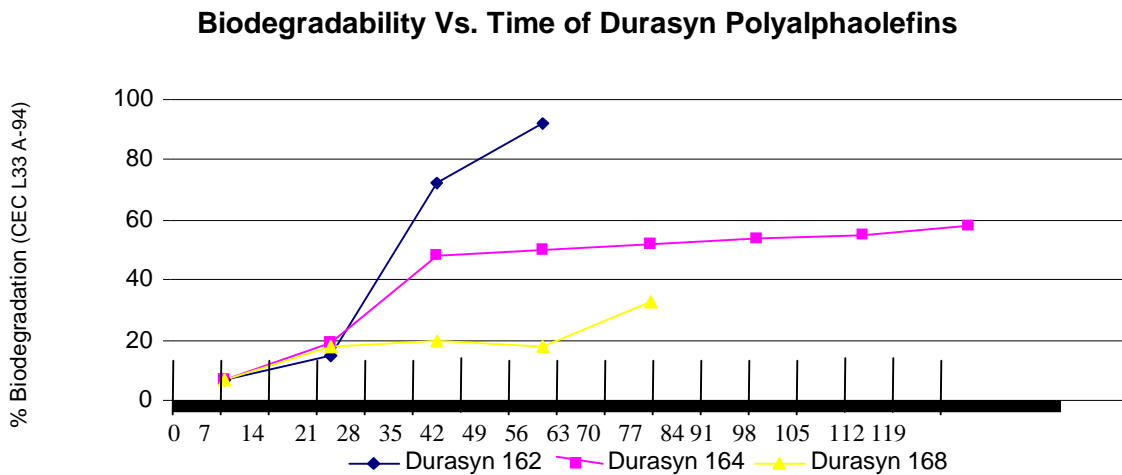
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**Durasyn<sup>®</sup> 162, 164 and 168 Polyalphaolefins continue to biodegrade throughout a time- extended CEC L33 A-94 experiment, well after the 21-day span prescribed in the standard method (Graph 3).**

Over time, Durasyn<sup>®</sup> 162, 164 and 168 Polyalphaolefins are not expected to persist in aquatic environments.

**Graph 3**



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## The CEC L33 A-94 Test for Biodegradability

The CEC L33 A-94 protocol was developed in Europe to determine the persistence of 2-stroke outboard engine oils in aquatic environments. In recent years, this test has been applied more broadly. In fact, it is fast becoming a standard in the lubricants industry for evaluating water-insoluble materials. Studies with lubricants<sup>5</sup> have shown a direct correlation between the results of the CEC test and actual persistence in the environment. Note that this test is not a test of “ready biodegradability” but one of “comparative biodegradability.” These terms are tightly defined by regulatory bodies.

The CEC L33 A-94 test procedure is summarized as follows. Test flasks (in triplicate) containing an aqueous mineral-salts medium, test oil, and inoculum, together with poisoned flasks, are incubated for 21 days. Flasks containing calibration materials (diisotridecyl adipate and white mineral oil) in the place of the test oil are run in parallel. At the end of the incubation times, the contents of the flasks are sonicated, acidified, and extracted with CCL<sub>4</sub> or R113 (1,1,2-trichlorotrifluoroethane). The extracts are then analyzed by IR spectroscopy, measuring the maximum absorption of the CH<sub>3</sub>-CH<sub>2</sub>-band at 2930 cm<sup>-1</sup>. The biodegradability is expressed as the % difference in residual oil content between the test flasks and the respective poisoned flasks at day 21.

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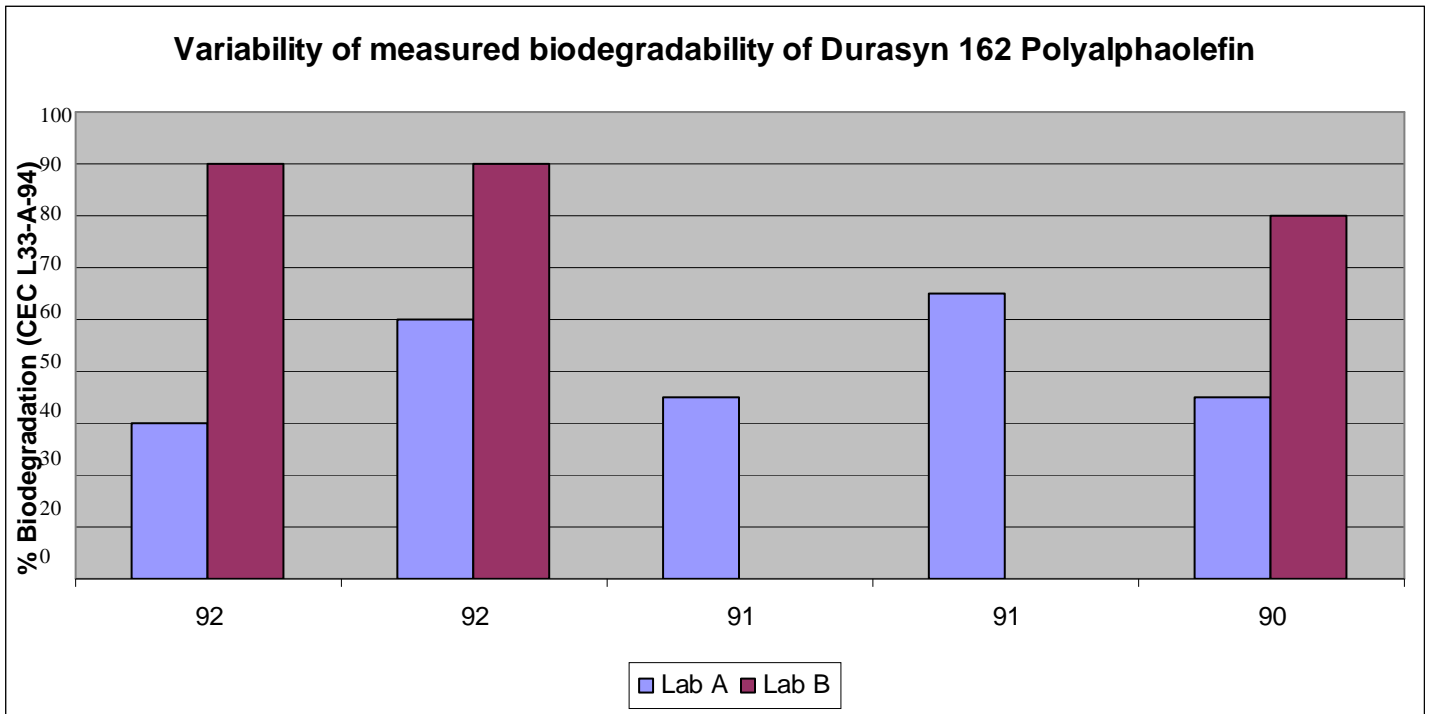
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Durasyn 162 Polyalphaolefin was tested repeatedly over a three-year period, and a range of values was obtained (see Graph 4). The different testing laboratories obtained their respective inocula at different times of the year from different municipal sewage treatment plants. This spread of values is not unexpected. Similar observations were noted with the other Durasyn Polyalphaolefins (see Graph 2).

The time-extended CEC L33 A-94 test involved longer time intervals before sacrificing the flasks. For each test material at each time interval, a set of replicate test flasks and poisoned flasks were sacrificed.

Graph 4



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## **Polyalphaolefins are not bioresistant.**

Durasyn<sup>®</sup> 162 through 170 Polyalphaolefins require biocides when used in metalworking fluid formulations. Without biocides, Polyalphaolefins exhibit no bioresistance when challenged with a mixed bacterial and fungal inoculum under aerobic conditions (A Modified ASTM method E686-85).

Tests for biodegradation and bioresistance measure similar phenomena: the former, degradation of substances by biotic processes; the latter, susceptibility of substances to microbial attack. In biodegradability tests, low levels of inoculum and nutrients are employed. These are the conditions that are anticipated for discharges into the normal environment. In bioresistance tests, high levels of inoculum and nutrients are employed. These highly favorable conditions are anticipated for specific sites, such as where metalworking fluids are used.

The bioresistance data clearly indicates that both the lower and the higher viscosity Durasyn Polyalphaolefins are prone to microbial attack.

## **BIOACCUMULATION**

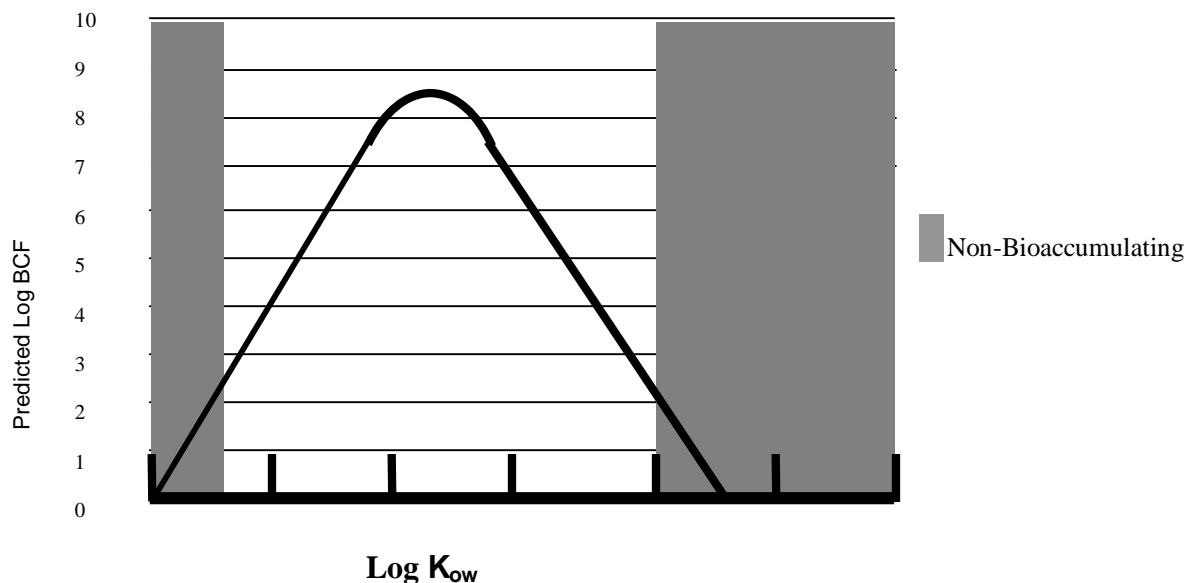
### **PAOs are not expected to bioaccumulate in aquatic species.**

Substances with both low and very high values of log  $K_{OW}$  are not expected to bioaccumulate in aquatic species.<sup>6,7</sup> The calculated log octanol/water partition coefficients for Polyalphaolefins are extraordinarily high, greater than 10.<sup>8</sup> In view of this, we do not expect PAOs to bioaccumulate in aquatic species.

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**Graph 5**  
**Relationship between Octanol / Water Partition**  
**Coefficient ( $\log K_{ow}$ ) and Bioconcentration**



<sup>6</sup>This relationship between  $\log K_{ow}$  and  $\log BCF$  is valid only for non-ionized organic chemicals.

<sup>7</sup> Droy, B. "Chapter 25: Environmental Impact" from Synthetic Lubricants and High Performance Functional Fluids R. L. Shubkin, ed., **1993**, Marcel Dekker, 533.

<sup>8</sup>PAOs'  $\log K_{ow}$  were also directly measured, by the ASTM have a  $\log K_{ow}$  greater than eight (8) which exceeds the upper limit of this test method.

<sup>9</sup> Leuterman, A.J.J.; Droy, B.F. Offshore **August 1991**, 66. McKim, J.; Schmieder, P.; Veith G. Toxicol. Appl. Pharmacol. **1985**, 77, 1. (U.S. Environmental Protection Agency, Environmental Research Laboratory)

<sup>10</sup> Until just recently, it was believed that a linear relationship existed between  $\log K_{ow}$  and  $\log BCF$ . Generally, all materials with  $\log K_{ow} > 3$  were categorized as bioaccumulators. Now, however, the roles of bioavailability and metabolism are being recognized.

<sup>11</sup> Bintein, S.; Devillers, J.; Karcher, W., "Nonlinear Dependence of Fish Bioconcentration on n-Octanol Partition Coefficients", SAR and SQAR in Env. Res. 1:29-30, 1993.

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## Bioconcentration and its relationship to the Octanol/Water Partition Coefficient

The bioconcentration factor (BCF) for aquatic organisms is defined as the ratio of the concentration of a material in an organism divided by that concentration of material found in the ambient aqueous phase. Like the LD<sub>50</sub>, the BCF of a material is used for environmental hazard assessment purposes. It is species-dependent and both difficult and costly to measure.

For aquatic species, a material's BCF can be estimated — as a first analysis — by its lipophilicity as quantified by its octanol/water partition coefficient ( $K_{OW}$ ).<sup>6</sup> The relationship between  $\log K_{OW}$  and  $\log BCF$  is well documented. Graph 5 illustrates that substances with either low or high values of  $\log K_{OW}$  are not expected to bioaccumulate in aquatic species.<sup>6,7,9,10,11</sup>

Materials with low values of  $\log K_{OW}$  are highly hydrophilic and are thus not expected to bioaccumulate. Instead, they are readily desorbed from the organism into the ambient aqueous medium.

Materials with very high values of  $\log K_{OW}$  have extremely low water solubility, and are thus not expected to bioaccumulate. In fact, they do not enter the organism in the first place. Passage through biological membranes (excluding active transport processes) requires that the material be available in a dissolved form in order to move past the aqueous diffusion layer at the interface. In effect, such materials are not biologically available.

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There are other reasons why materials with high values of  $\log K_{OW}$  are not expected to bioaccumulate. They are readily absorbed or partitioned onto suspended organic solids or into the organic fraction of the sediment. Thus, the material becomes either sequestered in the sediment or stuck to particles too large to pass through the biological membranes. In addition, Polyalphaolefins that have molecular weights greater than 600 are too large a molecule to move easily across membranes. The effect is the same; such materials are also not biologically available.

## **MATERIAL SAFETY DATA SHEETS / SAFETY DATA SHEETS**

Material Safety Data Sheets (MSDS /SDS) are available for all Durasyn® Polyalphaolefins, and describe the health, safety and environmental characteristics of these products as well as advice on handling precautions and emergency procedures.

MSDS should be consulted and fully understood before handling, storage or use of Durasyn® polyalphaolefins. To request a copy of a specific Durasyn® Polyalphaolefins grade Material Safety Data Sheet, phone 1-866-363-2454 Toll Free – (North America), +32 (0)67 875 980 (Europe), +86 21 6103 5970 (Asia), or send an e-mail to [oligomersmsds@ineos.com](mailto:oligomersmsds@ineos.com).

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