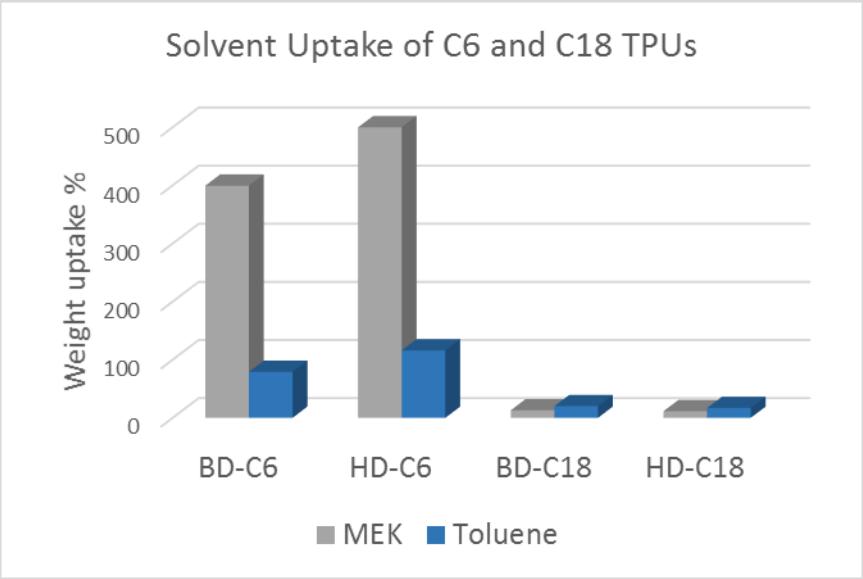
Product Bulletin

Elevance Inherent™ C18 Diacid

Product Application in Polyester Polyols

Elevance Inherent™ C18 Diacid is a long chain, linear, aliphatic diacid that can be used in the synthesis of polyester polyols. When incorporated into linear polymers, polyester polyols from Inherent™ C18 Diacid result in improved flexibility, lower moisture pickup, and increased hydrophobicity over polyols made from short or mid-chain diacids. The solvent resistance of TPUs based on polyester polyols from C18 diacid was tested in MEK and toluene; the results are shown in the figure below. TPUs based on C18 diacid are much more solvent resistant in polar solvents such as MEK and non-polar solvents such as toluene compared to TPUs based on adipic acid, which completely disintegrated upon exposure to these solvents.



Polyester polyols based on Inherent™ C18 Diacid can be used in thermoplastic or thermoset polyurethanes, in polyurethane foams, in thermoplastic elastomers, in adhesives and in polyester films and fibers. Additionally, a wide range of elasticity and hardness has been demonstrated in polyurethanes made from polyester polyols derived from Inherent™ C18 Diacid by varying the amount and type of the diisocyanate. These properties make polyurethanes based on Inherent™ C18 diacid versatile and robust materials that are suitable for demanding applications such as automotive undercarriage and fuel lines, hot melt adhesives, high performance coatings, and sports equipment.

Preparation of Polyester Polyols

We have used the following procedure in making polyester polyols from Inherent™ C18 Diacid and a typical diol, butane diol: A 1000 mL three neck round bottom flask was equipped with a magnetic stir bar, Dean-Stark adapter for water condensation, heating mantle, thermocouple, temperature controller, and a gas inlet for nitrogen to provide an inert nitrogen atmosphere. The neck of the Dean-Stark attachment was wrapped with heating tape and heated at ~105°C to facilitate water transport to the condenser. Condensed water, which is the product of esterification reaction, was collected in a glass flask placed below the condenser of the Dean Stark attachment.

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C18-diacid (Elevance Renewable Sciences, Inc.) in the amount of 373.3 g (1.19 moles) and 1,4, butanediol (Alfa Aesar) in the amount of 121.1 g (1.34 moles) were charged to a reaction flask and heated up to 120°C. At this temperature the reaction mixture was in a liquid phase and homogenized with agitation. Butyltintris (2-ethylhexanoate) catalyst (Chem Cruz) (0.07 g) dissolved in 1,4-butanediol (1.3 g) was then charged into the reaction mixture. An additional amount of 0.88 g of 1,4-BD was added to the reaction, which amounted to 2.18 g excess of 1,4-BD compared to the theoretical value of 121.1 g. The temperature of the reaction mixture was gradually increased to 170°C during 3-4 hours. The reaction took place under these conditions as indicated with significant water release. Afterwards, the reaction temperature was increased to 180°C and carried out until the acid number of the reaction reached 3.61 mg KOH/g and the water content was 0.022%.

The reaction mixture was cooled down to 120°C and degassed for two hours under vacuum ~10 mmHg. After degassing the temperature of the reaction mixture was increased to 180°C, an additional amount of 0.035 g of butyltintris (2-ethylhexanoate) catalyst was added and reaction was continued by monitoring the acid number until the acid number approached 1 mg KOH/g. At this point the temperature of the polyol was lowered to 120°C and left at that temperature for 16 hours under nitrogen blanket and continuous mixing. The polyol was discharged and analysis of the polyol carried out.
The properties of the resultant polyol are as follows:

Polyol Properties	Methods	Property
Acid number	ASTM D 4662 – 03	0.45
Hydroxyl number	ASTM D 4274 – 99	55.0
Moisture, %	ASTM D 4672-00 (Karl Fisher Titrator)	0.013
Viscosity at 90°C	ASTM D 4878-08 (Brookfield viscometer)	1550
Color	ASTM D 4890-03	Gardner color 2-3 Apha scale >500
Melting temperature, °C	ASTM D3418 Differential Scanning Calorimetry (DSC, Q 10, TA Instruments) at 10°C/min. cooling and heating rate	84

Handling Precautions

Product safety information required for this product is not included herein. Before handling, read material safety data sheet and container label for safe use, physical and health hazard information. The material safety data sheet is available from your local Elevance Renewable Sciences representative or may be available on the Elevance Renewable Sciences website at elevance.com.

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