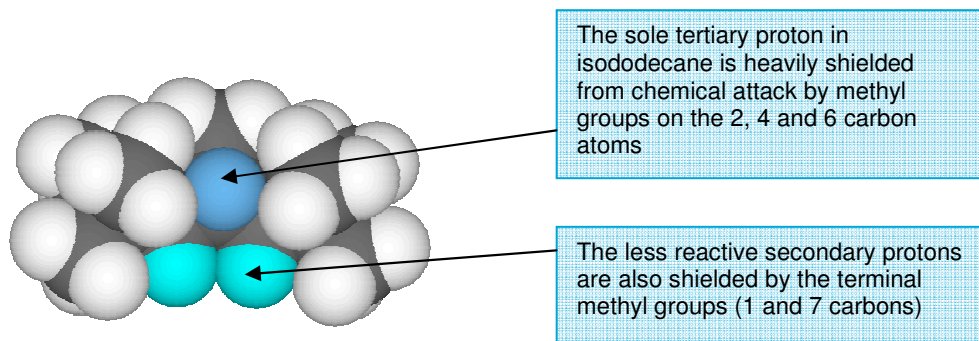


## Isododecane in the production of LDPE

Isododecane is an ultra pure, highly branched alkane, which is used extensively in radical catalysed polymerization reactions. It is the solvent / dispersant of choice for Europe's major producers of low-density polyethylene (LDPE), in both autoclave and tubular processes. Isododecane is used both as a carrier for peroxide catalysts, and a catalyst injection dispersant in the polymerization reaction itself. High activity peroxide catalysts used in the production of PVC and in cross-linked unsaturated polyester are also frequently dissolved in INEOS isododecane.

### Isododecane production and chemistry

Isododecane is produced by a patented process from a pre-purified isobutene (branched C4) containing feedstock, and is therefore totally synthetic. The name 'isododecane' is more a historical than a chemically correct term. In fact the structure of the main isomer in isododecane (2,2,4,6,6-pentamethylheptane, c.a. 83%) is close to a fully permethylated hydrocarbon structure (containing the maximum number of methyl groups). The dimethyl branches (termed as geminal, or gem dimethyls) in the isobutene monomer are retained in the final product, and it is this feature that makes isododecane so chemically resistant. Isododecane also contains approximately 17% of other pentamethylheptanes which have similar properties to the main isomer.



As a solvent / phlegmatizing agent in the production of LDPE initiator peroxides, resistance to oxidation is vital to ensure safe storage (increased SADT) and to prolong shelf life. Isododecane is used extensively for the most reactive (short half life) peroxide catalysts such as diacyl peroxides and peroxy diesters.

Chemical resistance is also important when isododecane is used as catalyst / initiator dispersant in LDPE production and the reaction conditions are even more severe. Even during the initiation stage of the reaction when the decomposing peroxide releases a high concentration of peroxy radicals isododecane remains totally inert. Analysis of the light post-reaction product has shown isododecane to be chemically unchanged.

### Purity and food contact

Solvent purity is critical for both polymer production, and for the properties and approvals of the finished product.

- The very high single isomer purity offered by INEOS isododecane ensures that in the reactor the product will behave exactly the same from batch to batch, helping to reduce potential process upsets.
- For grades where chain transfer agents are not used, aromatic impurities in the solvent are a special quality control headache. Isododecane is produced from isobutene, and the manufacturing chemistry prevents formation of any aromatics. This allows us to guarantee aromatics levels in isododecane of <1ppm, typically <0.2ppm.
- For packaging and especially film applications, food contact legislation compliance for polymer additives is essential. Isododecane is fully compliant with US polymer additive legislation (21 CFR §178.3530). In Europe, isododecane is classed as a polymerization aid and is excluded from the main food contact directive (2002/72/EC). INEOS has carried out a full risk assessment which shows that isododecane is safe for food contact applications with a very large margin of error. Isododecane is fully Kosher approved.
- Isododecane is free of all aromatic and naphthenic molecules, which ensures that the finished LDPE film will remain odour free. Single isomer purity allows residual traces of solvent to be easily detected by conventional means (e.g. gas chromatography).

### Contact information

#### Commercial

Angela Richter  
Tel. +44 (0) 2380 28 7316  
Fax.  
Mob. +44 (0) 7771661751  
E-Mail [angela.richter@innovene.com](mailto:angela.richter@innovene.com)

#### Technical

Dr Anthony Simoens  
Tel. +32 81 215700  
Fax. +32 81 215700  
Mob. +32 475 555 684  
E-mail [anthony.simoens@innovene.com](mailto:anthony.simoens@innovene.com)

INEOS web site

<http://www.ineosoligomers.com>

Technical documents can be downloaded directly from our technical services site (see hydrocarbons). By logging on, additional documents specific to your industry may be available.

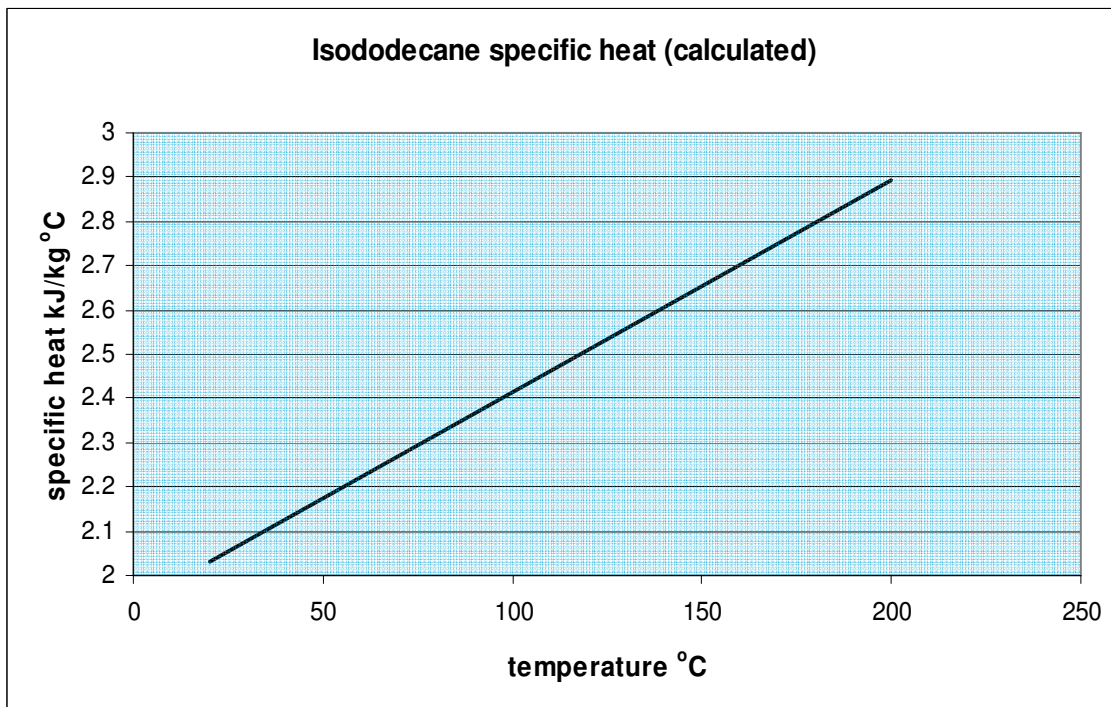
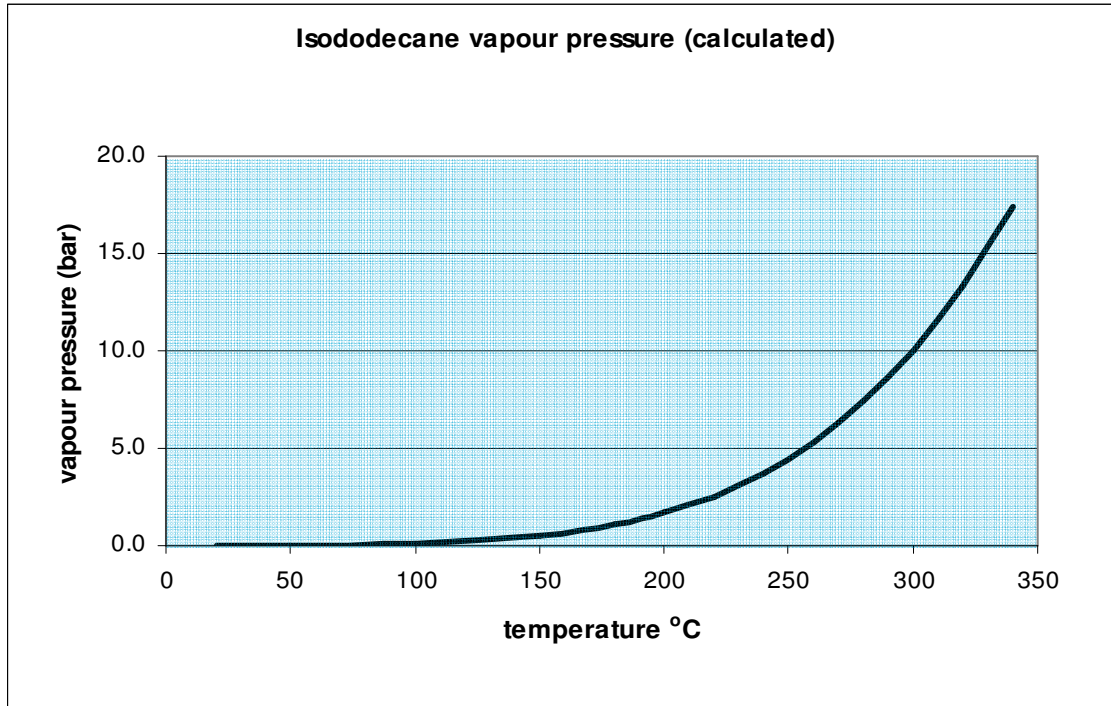
<http://www.innovene.com/technicalservices>

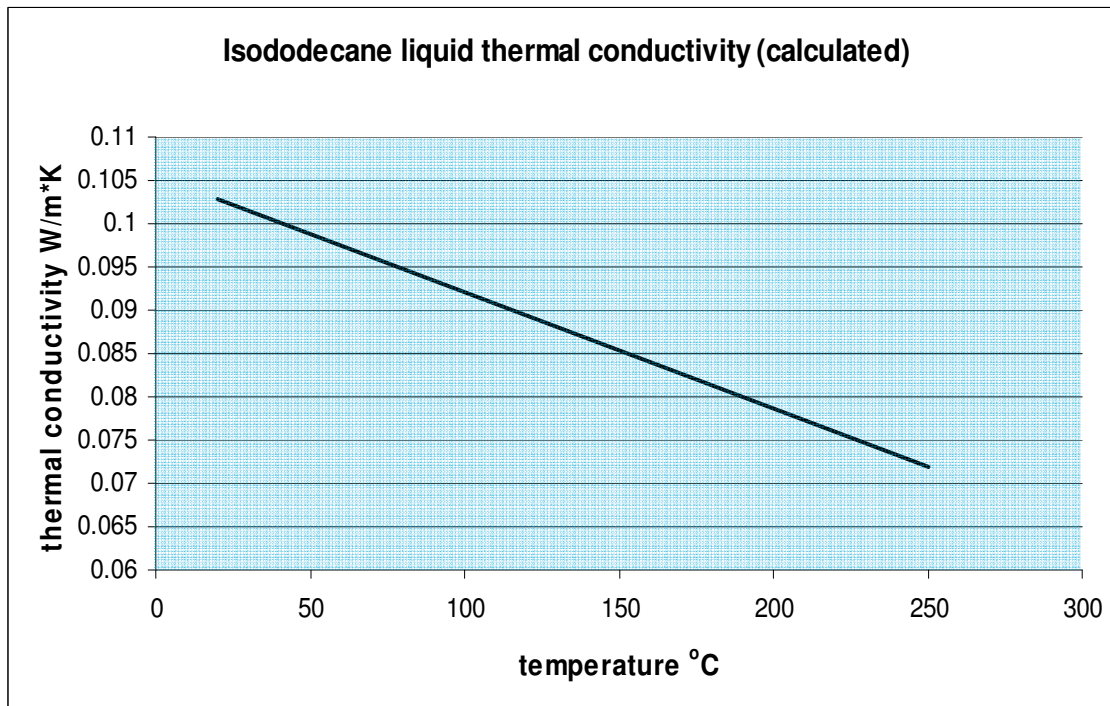
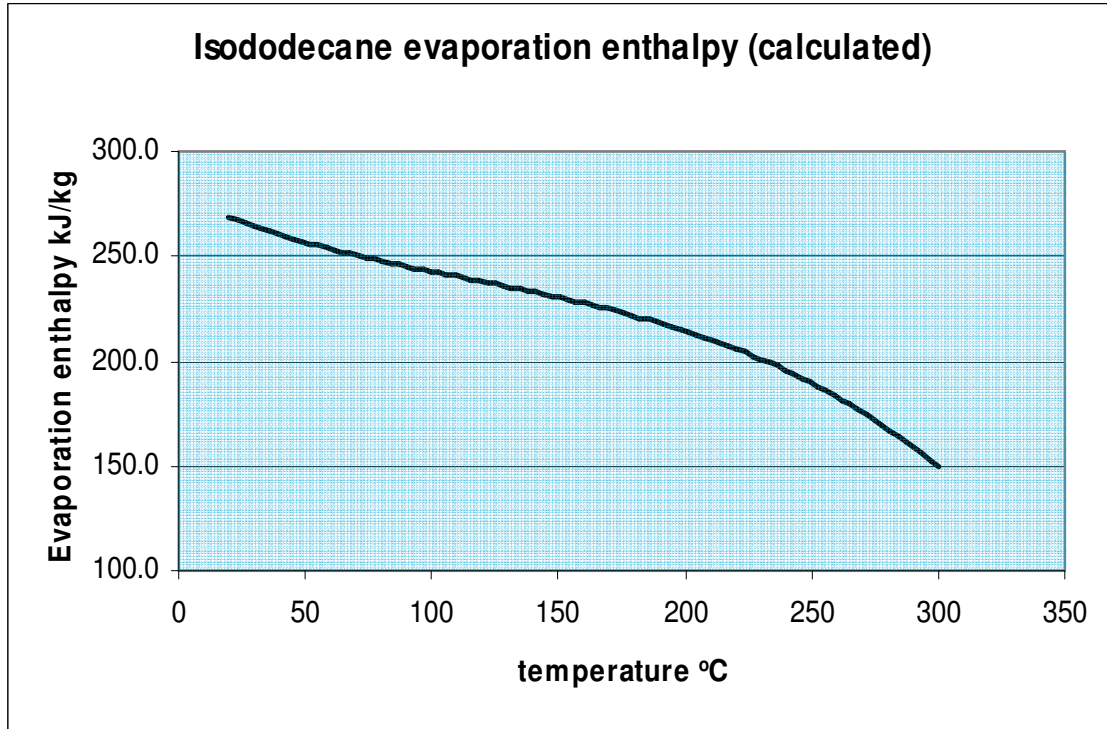
**Isododecane Sales Specification**

Parameter	Units	Value	Test Method
Sum of C <sub>12</sub> hydrocarbons	% by wt.	98 min	3002-0202103-98D (GC method)
Sum of C <sub>8</sub> and C <sub>16</sub> hydrocarbons	% by wt.	2 max	3002-0202103-98D (GC method)
Aromatics	mg/kg	1 max	3002-0600203-97D (UV method)
Carbonyls	mg/kg	5 max	3002-0300303-98D (titration)
Bromine index	mg Br <sub>2</sub> / 100g	15 max	3002-0300502-98D (potentiometric titration)
Sulphur	mg/kg	1 max	3002-0302802-00D (coulometric)
Peroxides (calculated as H <sub>2</sub> O <sub>2</sub> )	mg/kg	1 max	3002-0300502-98D (potentiometric titration)
Water	mg/kg	50 max	3002-0300101-95D (Karl Fischer titration)
Evaporation residue	mg/100ml	1 max	3002-0100201-95D (ASTM-D 381-80)
Neutralisation number	mg KOH/ g	0.01 max	3002-0300303-98D (titration)

**Isododecane Typical Properties**

Parameter	units	Conditions	Value
Boiling range start	°C		176
5% vol.	°C		179
95% vol.	°C		183
Boiling range end	°C		192
Flash point	°C		
Freezing point	°C		- 81
Density	g/ml	20 °C	0.75
Refractive index	n <sub>D</sub> <sup>20</sup>	20 °C	1.421 – 1.422
Dielectric constant		20 °C	2.12
Surface tension	mN/m	20 °C	22.6





**Isododecane Technical Safety Data**

Parameter	units	Conditions	Value
Autoignition temperature	°C		410
Ignition group			G2
Lower explosion limit	vol%		0.5
Upper explosion limit	vol%		4.0
Lower explosion point	°C		34
Upper explosion point	°C		73
Maximum explosion pressure	bar	1.4 vol%	4.2
Maximum rate of pressure increase (dp/dt)	bar	1.3 vol%	265
Relative vapour density		Air =1	5.9
Dielectric constant (20 °C)		2.12	

**September 2006**

**EXCLUSION OF LIABILITY**

INEOS Oligomers is a trading name for INEOS Europe Limited.  
 Information contained in this publication is accurate to the best of the knowledge and belief of INEOS Europe Ltd and its affiliates ("INEOS"). However, INEOS makes no representations or warranties express or implied, regarding the completeness, quality or accuracy of this information and any decisions you make based on the information contained herein are your sole responsibility.  
 Any information or advice obtained from INEOS otherwise than by means of this publication and whether relating to INEOS materials or other materials, is also given in good faith. However, it remains at all times the responsibility of the customer to ensure that INEOS materials are suitable for the particular purpose intended.  
 Insofar as materials not manufactured or supplied by INEOS are used in conjunction with or instead of INEOS materials, the customer should arrange to obtain from the manufacturer or supplier all technical data and other information relating to such materials.  
 Except as required by mandatory law, INEOS accepts no liability whatsoever arising out of the use of information supplied herein, the use of other materials in lieu of INEOS materials or the use of INEOS materials in conjunction with such other materials.

The name INEOS and the INEOS logo are trademarks of INEOS or its affiliated companies.  
 © 2006 INEOS  
 Sept 2006