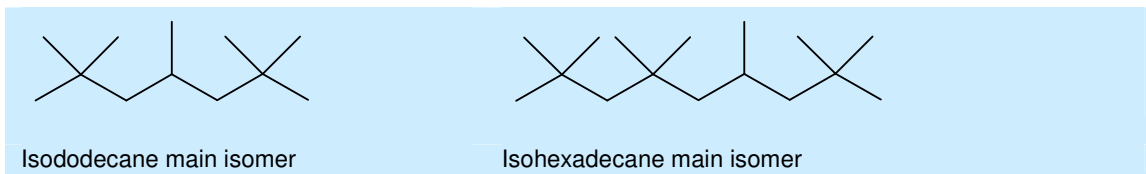


INEOS Isoalkanes in Cosmetics Formulation

The INEOS isoalkane range consists of isooctane (C_8), isododecane (C_{12}), isohexadecane (C_{16}) and isoicosane (C_{20}). They have been used extensively in a wide range of high performance cosmetics, generally providing the hydrophobic / lipophilic function in the formulation. With an excellent reputation in the cosmetics industry, they are well regarded for their high technical performance, high purity and dermatological compatibility.

Isoalkane production and chemical structure.

INEOS isoalkanes are produced by a patented process from a pre-purified isobutene (branched C_4) containing feedstock, and are therefore totally synthetic. From a chemists point of view, these molecules are actually much closer to a fully permethylated hydrocarbon structure (containing the maximum number of methyl groups) than the term 'isoalkane' would suggest. In particular, the dimethyl branches (geminal, or gem dimethyl) in the isobutene monomer are retained in the final product. It is this structural feature, together with carbon number and isomeric purities, which gives INEOS isoalkanes their unique physical properties.



In the first stage of the continuous production process, isobutene is oligomerized to give C_8 - C_{20} olefins. The relatively mild reaction conditions ensure that metathesis, positional isomerization and aromatization side reactions are suppressed. Further separation and hydrogenation of the reaction mixture provides the product isoalkanes. This lack of side reactions allows very high carbon number and isomeric purities to be achieved. For example, isododecane (typically >99.5% C_{12}) contains more than 80% of the single isomer, 2,2,4,6,6-pentamethylheptane. In contrast, isoalkanes produced from straight chain olefins (e.g. C_{11-13} isoalkanes) are carbon number mixtures containing hundreds to thousands of random branched isomers, and lack the characteristic gem dimethyl groups.

Technical performance

The permethylated structure makes INEOS isoalkanes hydrophobic to a degree not seen in other hydrocarbons, and gives them properties of particular value to the cosmetics formulator.

- Very high interfacial tensions with water allow robust Oil/Water and Water/Oil emulsions to be formed, with greater flexibility in the choice of emulsifiers, and potentially less problems with secondary additives. For non-drying isohexadecane and isoicosane, this property imparts excellent water resistance in fully formulated products
- Spreadability is a key property for emollients, especially for sun care products where a thin uniform film on the skin is vital for performance. INEOS isoalkanes exhibit unusually low contact angles and high spreadabilities, both in vitro and in vivo.

Fluid	Contact angle (°)	Spreading area (mm ² /4mg fluid)
Isohexadecane	0	1266
Isopropyl myristate	5	1044
Silicone 350	9	-
Mineral oil	15	661
Squalene	23	602
Castor oil	41	33

Literature results using simulated human skin

- INEOS isoalkanes are generally recognized as having attractive tactile properties, leaving a pleasant silky non-greasy feel on the skin. They are non-comedogenic

Purity and odour

INEOS's isoalkane range is designed to meet the high purity standards demanded by the modern cosmetics industry.

- Careful pre-treatment of the process feed is carried out to remove traces of aromatics and sulphur. Crucially, the unique reaction chemistry, (which prevents further aromatics/naphthenes formation), ensures that INEOS isoalkanes are completely free of aromatics, sulphur and naphthenes which might adversely affect odour and skin contact properties.
- Derived from petrochemical feedstocks, INEOSs isoalkanes are completely free of materials of animal and vegetable origin, and are therefore GMO, BSE and TSE compliant. Manufacturing practices eliminate the possibility of allergens and other harmful chemicals. INEOS's isoalkane range is fully Kosher accredited.
- Total metals content is typically less than 1ppm (part per million, or 1 mg/kg)

Stability and compatibility.

The gem dimethyl groups which characterize INEOS isoalkanes provide a high degree of steric hindrance, and make the molecules highly resistant to chemical attack, even under extreme conditions. We have determined that INEOS isoalkanes do not need the radical stabilizing agents sometimes added to less branched isoalkanes, although we would recommend that the peroxide content of very old product be checked before use, especially if containers have been exposed to the atmosphere. Samples of isododecane, for example, correctly stored in sealed containers showed no observable degradation even after seven years storage.

INEOS isoalkanes are of course completely immune to the hydrolysis reactions seen with fatty acid esters (e.g. isopropyl myristate and isopropyl palmitate), and are inert towards bases and non-oxidizing acids.

Silicones (polydimethylsiloxanes) share the gem dimethyl structure of the permethylated isoalkanes, which explains in part why INEOS isoalkanes make such good silicone viscosity cutters.

Availability

Our isoalkane range is only available directly from INEOS in bulk, generally full road tanks (c.a. 23MT), rail tanks or by ship. Smaller quantities and drummed material can be obtained through our distributor network.

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Technical documents can be downloaded directly from our technical services site, listed under the hydrocarbons section. By logging on, additional documents specific to your industry may be available.

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

Table 1. Properties of INEOS isoalkanes most widely used in cosmetics

Parameter	Units	°C	Isododecane	Isohexadecane	Isoeicosane
CAS number			93685-81-5 13475-82-6	93685-80-4 4390-04-9	93685-79-1
EINECS			297-629-8 236-757-0	297-628-2 224-506-8	297-627-7
Carbon number purity *	% by wt.		(C ₁₂) 98 min	(C ₁₆) 99 min.	(C ₂₀₊) 98 min
Minor paraffins *	% by wt.		(C ₈ /C ₁₆) 2 max	(C ₁₂ /C ₂₀) 1 max	(C ₁₆) 2 max.
Aromatics *	mg/kg		1 max	1 max	1 max
Carbonyls *	mg/kg		5 max	5 max	1 max.
Bromine no. *	mg Br ₂ /100g		15 max	500 max	2000 max
Sulphur *	mg/kg		1 max	1 max	5 max
Peroxides (as H ₂ O ₂) *	mg/kg		1 max	1 max	1 max
Water *	mg/kg		50 max	50 max	-
Initial boiling point	°C		176	241	275
Flash point	°C		50	101 min.*	> 130
Freezing point	°C		-81	-70	-49
Vapour pressure	mbar	20 30 50	4 7.4 20	2 - 9	- - -
Evaporation rate	Rel. Et ₂ O Rel. BuOAc		27 3	98 12	286 35
Viscosity	mPa*s	20	1.3	3.9	13.3
Density	g/cm ³	0 20 40	0.7618 0.7478 0.7334	0.7997 0.7867 0.7733	0.8233 0.8096 0.7967
Colour (Pt/Co)	Hazen		+2	+1	+2
Surface tension	mN/m	20	22.1	24.6	28.2
Solubility in water	ppm		0.04	<100	<100
Refractive index	n _D ²⁰	20 40	1.4201 1.4120	1.4405 1.4332	1.4512 1.4445
Aniline point	°C		+89	+95	-
Kauri butanol value			17.8	18.3	18.7
VOC content	%		100	0	0

* = specification item. All other values quoted are typical properties, and as such are not guaranteed

Cosmetic applications of INEOS isoalkanes.

As we are primarily a chemical manufacturer, INEOS does not offer detailed advice on cosmetics formulations. The table below is taken from public literature, and gives examples of the several hundred cosmetics and personal care products which have already been formulated with INEOS isoalkanes.

Product / property	Isododecane	Isohexadecane	Isoeicosane
INCI Name	Isododecane	Isohexadecane	Isoeicosane
Function	drying	Non-drying	
Decorative cosmetics	✓	✓	✓
Foundation creams		Non-greasy feel	
Make up removers	✓	✓	
Sun/skin care	✓	✓	✓
After / pre shaves	✓	✓	
Cologne / deodorants	✓	✓	
Antiperspirant sticks	✓	Lubricant / dispersant	
Deodorants	Emollient	Emollient	
Sprays / mousses	✓	Resin plasticizer	
Hair rinses, conditioners and mousses	✓	Conditioning agent	Resin plasticizer, luster finish
Mascaras	Solvent – low residual feel		Resin plasticizer
Lip creams		✓	
Pressed powders		Binder / emollient	

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