ISOPHORONE

Acronym : IPHO

• Synonym: 3,5,5-Trimethyl-2-cyclohexene-1-one

CAS number: 78-59-1EC number: 201-126-0

REACH registration number: 01-2119497282-32-0002

MAIN PROPERTIES

	Values	Arkema methods	Norms references
Composition	C9H14O:		
Appearance at 20°C	Clear liquid free from suspended materials	LCR 1116	ASTM D 4176
Color (Pt-Co)	≤ 50	LCR 1002	ASTM D 1209
Purity (isomers mixture*; % by weight)	≥ 99.0	LCR 2198	GC
Water Content (% by weight)	≤ 0.10	LCR 1007	ASTM D 1364
Acidity as acetic acid (% by weight)	≤ 0.01	LCR 1004	ASTM D 1613
Density at 20°C (g/cm³)	0.919 - 0.922	LCR 1062	ASTM D 4052

^{*} Isophorone consists essentially of 3,5,5-trimethyl-2-cyclohexene-1-one (α -isophorone or IPHO- α) in which less than 1 % of the isomer 3,5,5-trimethyl-3-cyclohexene-1-one (β -isophorone or IPHO- β) is present.

The above commercial specifications are guaranteed; they were established using the test methods which were in force at the plant at the time of despatch of the product, and are in accordance with any applicable revision references. (*) guaranteed values not reported on analysis certificates.

MAIN APPLICATIONS

- **Synthesis of IPDA and IPDI**: (isophorone diamine and isophorone diisocyanate) used in the manufacturing of epoxy, isocyanate and polyamide resins.
- Chemical synthesis: 3,5-xylenol, TMCHONE and TMCHOL (synthetic menthol) synthesis.
- **Pharmaceuticals:** Synthesis of Active Ingredients: Cyclonicate, Cyclandelate, Homosalate, Neramexane.
- Agrochemicals: Miscellaneous herbicide and insecticide formulations,.
- **Paints and varnishes:** Excellent solvent for PVDF resins. Levelling aid for polyacrylate, alkyde, epoxy, urea-formaldehyde, phenolic resins. Gloss properties.
- For further informations, please contact our technical services.



ISOPHORONE

PACKAGING

Isophorone is supplied in bulk by road tankers, isocontainers, IBC of net weight 870 kg, and in drums of net weight 195 kg.

STORAGE / SAFETY / PRECAUTIONS DURING USE / HANDLING

Please refer to the safety data sheet before any use. Typical shelf life at 25°C is 12 months with a possible color evolution.

PHYSICAL DATA

Molecular weight	138.21
Molecular weight	215.2 °C
Vapor pressure at 20°C	0.4 hPa
Relative evaporation rate (n-butyl acetate = 1)	0.04
Freezing point	- 8.1 °C
Viscosity at 20°C	2.6 mPa.s
Surface tension at 20°C	32.3 mN/m
Refractive index at 20 °C	1.4780
Latent heat of vaporization	307 kJ/kg
Specific heat (liquid at 20°C)	1.81 kJ/kg/K
Heat of combustion at 25°C	35690 kJ/kg
Flash point (closed cup)	85 °C
Autoignition temperature	462 °C
Explosivity limits in air (lower / upper)	0.8 / 3.8 % (v/v)
Electrical conductivity at 25 °C	0.36 μS/m
Solubility at 20 °C: - IPHO in water (mass fraction)	1.2 %
- water in IPHO (mass fraction)	4.3 %
Azeotrope with water : - boiling point at 1013 hPa	99.5 °C
- water content (% w/w)	83.9 %
Hansen solubility parameters at 25°C (∂t, ∂d, ∂p, ∂h)	19.9 / 16.6 / 8.2 / 7.4 MPa ^{1/2}

Updated: January 8, 2020 Revision: 3 File n°: 30.GA.10.2013

The statements, technical information and recommendations contained herein are believed to be accurate as of the date hereof. Since the conditions and methods of use of the product and of the information referred to herein are beyond our control, ARKEMA expressly disclaims any and all liability as to any results obtained or arising from any use of the product or reliance on such information; NO WARRANTY OF FITNESS FOR ANY PARTICULAR PURPOSE, WARRANTY OF MERCHANTABILITY OR ANY OTHER WARRANTY, EXPRESS OR IMPLIED, IS MADE CONCERNING THE GOODS DESCRIBED OR THE INFORMATION PROVIDED HEREIN. The information provided herein relates only to the specific product designated and may not be applicable when such product is used in combination with other materials or in any process. The user should thoroughly test any application before commercialization. Nothing contained herein constitutes a license to practice under any patent and it should not be construed as an inducement to infringe any patent and the user is advised to take appropriate steps to be sure that any proposed use of the product will not result in patent infringement.

This grade is suitable for many different applications. Therefore, any use of our grade as finished products intended to be used in specific markets including but not limited to drinking water treatment, cosmetics, pharmaceuticals products, food additives is under the sole responsibility of the Client. The Client must assume all risks and liability in connection herewith.

See MSDS for Health & Safety Considerations

