Shell Chemicals

Isohexane

TECHNICAL DATASHEET

Special Boiling Point Solvents
SICC Product Code: Q1215
CAS Registry Number: 64742-49-0
EC Number: 931-254-9

Description

Isohexane is a narrow boiling range, C_6 hydrocarbon solvent with a n-Hexane content of less than 3.5%. Being made from hydrogenated feedstock, its aromatics and olefins content is very low.

Typical Physical Properties

Property	Unit	Value	Method
Density @ 15°C	**kg/l**	**0.663**	**ASTM D4052**
Coefficient of Cubic Expansion @ 20°C	**10^{-4}**	**14**	**calculated**
Refractive Index @ 20°C	**-**	**1.374**	**ASTM D1218**
Colour	**Saybolt**	**+30**	**ASTM D156**
Bromine index	**mg Br/100g**	**< 5**	**ASTM D2710**
Copper Corrosion (1hr @ 100°C)	**-**	**1**	**ASTM D130**
Doctor Test	**-**	**Negative**	**ASTM D4952**
Non-Volatile Matter	**mg/100 ml**	**< 1**	**ASTM D1353**
Distillation, Initial Boiling Point	**°C**	**59**	**ASTM D1078**
Distillation, Dry Point	**°C**	**63**	**ASTM D1078**
Relative Evaporation rate (nBuAc=1)	**-**	**9.4**	**ASTM D3539**
Antoine Constant A#	**kPa, °C**	**7.68550**	**-**
Antoine Constant B#	**kPa, °C**	**2322.21**	**-**
Antoine Constant C#	**kPa, °C**	**349.110**	**-**

Notes:

#: In the Antoine temperature range, the vapor pressure P (kPa) at temperature T (°C) can be calculated by means of the Antoine equation: log P = A – B/(T+C).

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Typical Physical Properties

Property	Unit	Value	Method
Antoine Constants: Temperature range	°C	0 to +55	-
Vapor Pressure @ 0°C	kPa	11	Calculated
Vapor Pressure @ 20°C	kPa	25	Calculated
Saturated Vapor Concentration @ 20°C	g/m^3	875	Calculated
Paraffins	%m/m	97	GC
Napthenes	%m/m	3	GC
Aromatics	mg/kg	< 5	SMS 2728
Benzene	mg/kg	< 3	GC
n-Hexane	%m/m	3	GC
Sulfur	mg/kg	< 0.5	ISO 20846
Flashpoint (Abel)	°C	-47	IP170
Lower Explosion Limit in Air	%v/v	1.0	
Upper Explosion Limit in Air	%v/v	7.4	
Auto Ignition Temperature	°C	405	ASTM E659
Electric Conductivity @ 20°C	pS/m	< 1	ASTM D4308
Dielectric Constant	-	1.8	-
Pour Point	°C	< -50	ASTM D97
Viscosity @ 25°C	mm^2/s	0.43	ASTM D445
Surface Tension @ 20°C	mN/m	17	Du Nouy ring
Thermal Conductivity @ 20°C	W/m/°C	0.12	-
Hildebrand Solubility Parameter	$(cal/cm^3)^{1/2}$	7.2	
Hydrogen Bonding Index	-	0	-
Fraction Polarity	-	0	-
Heat of Vaporization at T_{boil}	kJ/kg	342	-
Heat of Combustion (Net) @ 25°C	kJ/kg	46000	-
Specific Heat @ 20°C	kJ/kg/°C	2.2	-
Molecular Weight	g/mol	86	Calculated

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Test Methods

Copies of copyrighted test methods can be obtained from the issuing organisations:

- American Society for Testing and Materials (ASTM)
- International Organization for Standardization (ISO)
- Deutsches Institut für Normung (DIN)

Shell Method Series (SMS) methods are issued by Shell Global Solutions International B.V., Shell Technology Centre, Amsterdam, The Netherlands. Requests for copies of SMS can be made through your local Shell Chemicals company.

N.B: For routine quality control local test methods may be applied. Such methods have been validated against those mentioned in this datasheet.

Quality

Isohexane does not contain detectable quantities of polycyclic aromatics, heavy metals or chlorinated compounds.

Hazard Information

For detailed Hazard Information please refer to the Safety Data Sheet.

Access Safety Data Sheets here: Safety Data Sheets

Storage and Handling

Provided proper storage and handling precautions are taken we would expect Isohexane to be technically stable for at least 12 months. For detailed advice on Storage and Handling please refer to the Safety Data Sheet

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