Shell Chemicals

Heptane

TECHNICAL DATASHEET

Special Boiling Point Solvent
SICC Product Code: Q1352
CAS Registry Number: 64742-49-0
EC Number: 927-510-4

Description

Heptane is a narrow boiling range C7 hydrocarbon solvent, low in n-hexane. Being made from hydrogenated feedstock, its aromatics and olefins content is very low.

Typical Chemical Properties – Heptane

Property	Unit	Value	Method
Density @ 15°C	**kg/l**	**0.721**	**ASTM D4052**
Coefficient of Cubic Expansion @ 20°C	**10^{-4}**	**13**	**calculated**
Refractive Index @ 20°C	**-**	**1.401**	**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**	**95**	**ASTM D1078**
Distillation, Dry Point	**°C**	**99**	**ASTM D1078**
Relative Evaporation rate (nBuAc=1)	**-**	**3.9**	**ASTM D3539**
Antoine Constant A#	**kPa, °C**	**7.72070**	**-**
Antoine Constant B#	**kPa, °C**	**2545.47**	**-**
Antoine Constant C#	**kPa, °C**	**349.430**	**-**

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).

Shell Chemicals

Typical Physical Properties – Heptane

Property	Unit	Value	Method
Antoine Constants: Temperature range	°C	+30 to +90	-
Vapor Pressure @ 0°C	kPa	2.7	Calculated
Vapor Pressure @ 20°C	kPa	6.8	Calculated
Saturated Vapor Concentration @ 20°C	g/m^3	275	Calculated
Paraffins	%m/m	60	GC
Napthenes	%m/m	40	GC
Aromatics	mg/kg	< 5	SMS 2728
Benzene	mg/kg	< 3	GC
n-Hexane	%m/m	< 0.1	GC
n-Heptane	%m/m	> 30	GC
Sulfur	mg/kg	< 0.5	ISO 20846
Flashpoint, (Abel)	°C	-7	IP170
Lower Explosion Limit in Air	%v/v	1.0	
Upper Explosion Limit in Air	%v/v	7.0	
Auto Ignition Temperature	°C	215	ASTM E659
Electric Conductivity @ 20°C	pS/m	< 1	ASTM D4308
Dielectric Constant	-	1.9	-
Pour Point	°C	< -50	ASTM D97
Viscosity @ 25°C	mm^2/s	0.64	ASTM D445
Surface Tension @ 20°C	mN/m	21	Du Nouy ring
Thermal Conductivity @ 20°C	W/m/°C	0.12	-
Hildebrand Solubility Parameter	$(cal/cm^3)^{1/2}$	7.5	
Hydrogen Bonding Index	-	0	-
Fraction Polarity	-	0	-
Heat of Vaporization at T_{boil}	kJ/kg	315	-
Heat of Combustion (Net) @ 25°C	kJ/kg	45500	-
Specific Heat @ 20°C	kJ/kg/°C	2.1	-
Molecular Weight	g/mol	99	Calculated

Shell Chemicals

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

Heptane 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 Heptane to be technically stable for at least 12 months. For detailed advice on Storage and Handling please refer to the Safety Data Sheet

Shell Warranties

All products purchased or supplied by Shell chemicals companies are subject to the terms and conditions set out in the contract, order confirmation and/or bill of lading. All other information supplied by Shell chemicals companies, including that herein, is considered accurate but is furnished upon the express condition that the customer shall make its own assessment to determine a product's suitability for a particular purpose. Except as may be set forth in the applicable contract, order confirmation and/or bill of lading, Shell chemicals companies make no warranty, express or implied, including regarding any information supplied or the data upon which it is based or the results to be obtained from the use of such products or information, or concerning product, whether of satisfactory quality, merchantability, fitness for any particular purpose or otherwise, or with respect to intellectual property infringement as a result of use of information or products, and none shall be implied.

Shell Chemicals

The expression ‘Shell Chemicals’ refers to the companies of Shell Plc./Shell Group that are engaged in chemical businesses. Each of the companies that make up Shell Plc./Shell Group of companies is an independent entity and has its own separate identity.

Learn more at www.shell.com/chemicals