Shell Chemicals



Technical Datasheet

Heptane

Product Code Q1352

Region Europe

Product Category Special Boiling Point Solvents

CAS Registry Number 64742-49-0

EINECS Number 265-151-9

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 Properties

Property	Unit	Method	Value
Water	% m/m	ASTM D1364	< 0.005
Density @15°C	kg/L	ASTM D4052	0.717
Coefficient of Cubic Expansion @20°C	10 ⁻⁴ /°C	Calculated	13
Refractive Index @20°C	-	ASTM D1218	1.399
Colour	Saybolt	ASTM D156	+30
Bromine Index	mg Br/100g	ASTM D1492	< 5
Copper Corrosion (1hr @100°C)	-	ASTM D130	1
Doctor Test	-	ASTM D4952	Negative
Non Volatile Matter	mg/100ml	ASTM D1353	1
Distillation, Initial Boiling Point	°C	ASTM D1078	95
Distillation, Dry Point	°C	ASTM D1078	99
Relative Evaporation Rate (nBuAc=1)	-	ASTM D3539	3.9
Relative Evaporation Rate (Ether=1)	-	DIN 53170	3.0
Antoine Constant A #	kPa, °C	-	7.72070
Antoine Constant B #	kPa, °C	-	2545.47
Antoine Constant C #	kPa, °C	-	349.430
Antoine Constants: Temperature range	°C	-	+30 to +90

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Vapor Pressure @ 0°C	kPa	Calculated	2.7
Vapor Pressure @ 20°C	kPa	Calculated	6.8
Saturated Vapor Concentration @ 20°C	g/m³	Calculated	275
Paraffins	% m/m	GC	70
Naphthenes	% m/m	GC	30
Aromatics	mg/kg	SMS 2728	< 5
Benzene	mg/kg	GC	< 3
n-Hexane	%m/m	GC	< 0.1
n-Heptane	% m/m	GC	39
Sulfur	mg/kg	ISO 20846	< 0.5
Flash Point, (Abel)	°C	IP170	-7
Lower Explosion Limit in Air	% v/v		1.0
Upper Explosion Limit in Air	% v/v		7.0
Auto Ignition Temperature	°C	ASTM E659	215
Electrical Conductivity @ 20°C	pS/m	ASTM D4308	< 1
Dielectric Constant @ 20°C	-	-	1.9
Aniline Point	°C	ASTM D611	61
Kauri-Butanol Value	-	ASTM D1133	32
Pour Point	°C	ASTM D97	< -50
Viscosity @ 25°C	mm ² /s	ASTM D445	0.64
Surface Tension @20°C	mN/m	Du Nouy ring	21
Thermal Conductivity @ 20°C	W/m/°C		0.12
Hildebrand Solubility Parameter	(cal/cm ³) ^{1/2}	-	7.5
Hydrogen Bonding Index	-	-	0
Fractional Polarity	-	-	0
Heat of Vaporization at T _{boil}	kJ/kg	-	315
Heat of Combustion (Net) @t 25°C	kJ/kg	-	45500
Specific Heat @ 20°C	kJ/kg/°C	-	2.1
Molecular Weight	g/mol	Calculated	99

^(#) 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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Test Methods

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

American Society for Testing and Materials (ASTM) : www.astm.org International Organization for Standardization (ISO) : www.iso.org Deutsches Institut für Normung (DIN) : www.din.de

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 on www.shell.com/chemicals.

Storage 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 on www.shell.com/chemicals.

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