Shell Chemicals

Technical Datasheet

Hexane Polymerisation

Product Code	Q1241
Region	Europe
Product Category	Special Boiling Point Solvents
CAS Registry Number	64742-49-0
EINECS Number	265-151-9
Description	Hexane Polymerisation Grade is manufactured to the high standards required by the polymerisation industry. The solvent contains about 50% n-hexane, with a similar content of other hexane isomers. It is very low in impurties such as aromatics, olefins, carbonyls and acid substances.

Typical Properties

Property	Unit	Method	Value
Water	% m/m	ASTM D1364	< 0.005
Density @15°C	kg/L	ASTM D4052	0.676
Coefficient of Cubic Expansion @20°C	10^{-4}/°C	Calculated	13
Refractive Index @20°C	-	ASTM D1218	1.380
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	< 0.5
Distillation, Initial Boiling Point	°C	ASTM D1078	66
Distillation, Dry Point	°C	ASTM D1078	70
Relative Evaporation Rate (nBuAc=1)	-	ASTM D3539	8.0
Relative Evaporation Rate (Ether=1)	-	DIN 53170	1.4
Antoine Constant A #	kPa, °C	-	7.38070
Antoine Constant B #	kPa, °C	-	2110.27
Antoine Constant C #	kPa, °C	-	326.200

Antoine Constants: Temperature range	°C	-	+20 to +70
Vapor Pressure @ 0°C	kPa	Calculated	8.2
Vapor Pressure @ 20°C	kPa	Calculated	19
Saturated Vapor Concentration @ 20°C	g/m^3	Calculated	681
Paraffins	% m/m	GC	85
Naphthenes	% m/m	GC	15
Aromatics	mg/kg	SMS 2728	< 5
Benzene	mg/kg	GC	< 3
n-Hexane	%m/m	GC	50
Sulfur	mg/kg	ISO 20846	< 0.5
Flash Point, (Abel)	°C	IP170	< -30
Lower Explosion Limit in Air	% v/v		1.1
Upper Explosion Limit in Air	% v/v		7.4
Auto Ignition Temperature	°C	ASTM E659	375
Electrical Conductivity @ 20°C	pS/m	ASTM D4308	< 1
Aniline Point	°C	ASTM D611	65
Kauri-Butanol Value	-	ASTM D1133	31
Pour Point	°C	ASTM D97	< -50
Viscosity @ 25°C	mm^2/s	ASTM D445	0.49
Surface Tension @20°C	mN/m	Du Nouy ring	19
Thermal Conductivity @ 20°C	W/m/°C		0.12
Hildebrand Solubility Parameter	$(cal/cm^3)^{1/2}$	-	7.3
Hydrogen Bonding Index	-	-	0
Fractional Polarity	-	-	0
Heat of Vaporization at T_{boil}	kJ/kg	-	333
Heat of Combustion (Net) @t 25°C	kJ/kg	-	46000
Specific Heat @ 20°C	kJ/kg/°C	-	2.2
Molecular Weight	g/mol	Calculated	86

(#) 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)

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

Hexane Polymerisation Grade can be supplied to meet the requirements of ASTM D1836.
Hexane Polymerisation Grade 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 ww.shell.com/chemicals.

Storage Handling

Provided proper storage and handling precautions are taken we would expect Hexane Polymerisation Grade 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.