



# Diisobutyl Ketone

<b>Product Code</b>	S1226
<b>Region</b>	Asian Pacific
<b>Product Category</b>	Ketones
<b>CAS Registry Number</b>	108-83-8
<b>Synonym(s)</b>	DIBK; isovalerone; 2,6[4,6]-dimethyl-4[2]-heptanone
<b>Description</b>	Diisobutyl ketone is a slow evaporating ketonic solvent which is immiscible with water, but miscible with other organic solvents. It is a light coloured liquid with a mild, characteristic odour. Shell DIBK is a mixture of two isomers: 2,6-dimethyl-4-heptanone and 4,6-dimethyl-2-heptanone in the ratio 2:1.

## Typical Properties

Property	Unit	Method	Value
Purity, min.	%m/m	GC	94.0
Water	%m/m	ASTM D1364	0.03
Density at 20°C	kg/l	ASTM D4052	0.808
Specific Gravity at 20°C/20°C	-	ASTM D4052	0.810
Specific Gravity at 25°C/25°C	-	ASTM D4052	0.806
Coefficient of Cubic Expansion at 20°C	10 <sup>-4</sup> /°C	Calculated	10
Refractive Index at 20°C	-	ASTM D1218	1.413
Colour	Pt-Co	ASTM D1209	< 20
Boiling Point	°C	-	168
Relative Evaporation Rate (nBuAc=1)	-	ASTM D3539	0.18
Relative Evaporation Rate (Ether=1)	-	DIN 53170	48
Antoine Constant A #	kPa. °C	-	6.07029
Antoine Constant B #	kPa. °C	-	1476.40
Antoine Constant C #	kPa. °C	-	195.000
Temperature Limits for Antoine Equation #	°C	-	+20 to +170
Vapour Pressure at 20°C	kPa	Calculated	0.16

Vapour Pressure at 50°C	kPa	Calculated	1.1
Saturated Vapor Concentration at 20°C	g/m <sup>3</sup>	Calculated	9
Volatile Organic Compound (VOC)	g/l	EU / EPA	808
Flash Point (Abel)	°C	IP 170	50
Auto Ignition Temperature	°C	ASTM E659	345
Lower Explosion Limit	%v/v	-	0.8
Upper Explosion Limit	%v/v	-	6.2
Electrical Conductivity at 20°C	pS/m	ASTM D4308	4*10 <sup>6</sup>
Dielectric Constant at 20°C	-	-	9.9
Freezing Point	°C	-	-42
Surface Tension at 20°C	mN/m	-	23
Viscosity at 20°C	mPa.s	-	0.92
Hildebrand Solubility Parameter	(cal/cm <sup>3</sup> ) <sup>1/2</sup>	-	7.8
Hydrogen Bonding Index	-	-	9.8
Fractional Polarity	-	-	0.123
Heat of Vaporisation at T <sub>boil</sub>	kJ/kg	-	277
Heat of Combustion (Net) at 25°C	kJ/kg	-	37500
Specific Heat at 20°C	kJ/kg/°C	-	1.96
Thermal Conductivity at 20°C	W/m/°C	-	0.13
Miscibility at 20°C: Solvent in water	%m/m	-	0.05
Miscibility at 20°C: Water in solvent	%m/m	-	0.45
Azeotrope with Water: Boiling Point	°C	-	97.3
Azeotrope with Water: Solvent Content	%m/m	-	49.0
Molecular Weight	g/mol	-	142

(#) 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](http://www.astm.org)  
Energy Institute (IP) : [www.energyinst.org.uk](http://www.energyinst.org.uk)  
Deutsches Institut für Normung (DIN) : [www.din.de](http://www.din.de)

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

## Quality

Diisobutyl Ketone 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](http://www.shell.com/chemicals).

## Storage Handling

Provided proper storage and handling precautions are taken we would expect Diisobutyl Ketone 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](http://www.shell.com/chemicals).

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.

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