Diisobutyl Ketone

Product Code: S1226
Region: Asian Pacific
Product Category: Ketones
CAS Registry Number: 108-83-8
Synonym(s): DIBK; isovalerone; 2,6[4,6]-dimethyl-4[2]-heptanone
Description: 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

<table>
<thead>
<tr>
<th>Property</th>
<th>Unit</th>
<th>Method</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Purity, min.</td>
<td>%m/m</td>
<td>GC</td>
<td>94.0</td>
</tr>
<tr>
<td>Water</td>
<td>%m/m</td>
<td>ASTM D1364</td>
<td>0.03</td>
</tr>
<tr>
<td>Density at 20°C</td>
<td>kg/l</td>
<td>ASTM D4052</td>
<td>0.808</td>
</tr>
<tr>
<td>Specific Gravity at 20°C/20°C</td>
<td>-</td>
<td>ASTM D4052</td>
<td>0.810</td>
</tr>
<tr>
<td>Specific Gravity at 25°C/25°C</td>
<td>-</td>
<td>ASTM D4052</td>
<td>0.806</td>
</tr>
<tr>
<td>Coefficient of Cubic Expansion at 20°C</td>
<td>10⁻⁴/°C</td>
<td>Calculated</td>
<td>10</td>
</tr>
<tr>
<td>Refractive Index at 20°C</td>
<td>-</td>
<td>ASTM D1218</td>
<td>1.413</td>
</tr>
<tr>
<td>Colour</td>
<td>Pt-Co</td>
<td>ASTM D1209</td>
<td>&lt; 20</td>
</tr>
<tr>
<td>Boiling Point</td>
<td>°C</td>
<td>-</td>
<td>168</td>
</tr>
<tr>
<td>Relative Evaporation Rate (nBuAc=1)</td>
<td>-</td>
<td>ASTM D3539</td>
<td>0.18</td>
</tr>
<tr>
<td>Relative Evaporation Rate (Ether=1)</td>
<td>-</td>
<td>DIN 53170</td>
<td>48</td>
</tr>
<tr>
<td>Antoine Constant A</td>
<td>kPa. °C</td>
<td>-</td>
<td>6.07029</td>
</tr>
<tr>
<td>Antoine Constant B</td>
<td>kPa. °C</td>
<td>-</td>
<td>1476.40</td>
</tr>
<tr>
<td>Antoine Constant C</td>
<td>kPa. °C</td>
<td>-</td>
<td>195.000</td>
</tr>
<tr>
<td>Temperature Limits for Antoine Equation</td>
<td>°C</td>
<td>-</td>
<td>+20 to +170</td>
</tr>
<tr>
<td>Vapour Pressure at 20°C</td>
<td>kPa</td>
<td>Calculated</td>
<td>0.16</td>
</tr>
</tbody>
</table>
### Vapour Pressure at 50°C
- **kPa**
- **Calculated**: 1.1

### Saturated Vapor Concentration at 20°C
- **g/m³**
- **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**: $4 \times 10^6$

### 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/cm³)¹/²**
- **-**: 7.8

### Hydrogen Bonding Index
- **-**
- **-**: 9.8

### Fractional Polarity
- **-**
- **-**: 0.123

### Heat of Vapourisation 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

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**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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**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.

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.

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