2,2,4,4-Tetramethyl Pentane (TMP)  
Physical Properties and Safety Considerations for Use as a Calorimeter Fluid  

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1. Properties of N-Nonane and Its Isomers

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1.0 INTRODUCTION

Tetra Methylpentane, or TMP, has been proposed as a detector working fluid for the forward calorimeters of possible detectors. It has the empirical formula C_{9}H_{20}, is an isomer of nonane, and has the structure:

\[
\begin{align*}
\text{CH}_3 & \quad \text{CH}_3 \\
\text{CH}_3 & \quad \text{C} \quad \text{CH}_2 \quad \text{C} \quad \text{CH}_3 \\
\text{CH}_3 & \quad \text{CH}_3
\end{align*}
\]

TMP

There is some information and misinformation available about this compound, but overall its properties are estimated by similarity. It is between N nonane and isooctane, and a body of information is available for both of these common compounds. This report is intended to gather the safety-related information developed for 2,2,4,4-tetramethyl pentane into one place and to point out and eliminate misconceptions encountered.

2.0 GENERAL DESCRIPTION

TMP is a combustible liquid, very similar to gasoline, at room temperature and conditions. It is one of the isomers of nonane, and is only one CH\text{2} group different from isooctane, shown below, the key compound for which the gasoline octane rating is named.

\[
\begin{align*}
\text{CH}_3 & \quad \text{CH}_3 \\
\text{CH}_3 & \quad \text{C} \quad \text{C} \quad \text{CH}_3 \\
\text{CH}_3 & \quad \text{CH}_3
\end{align*}
\]

isooctane

There are 35 isomers of nonane (listed below) and even more isomers of decane and higher hydrocarbon compounds. It has been impossible to do a complete characterization of all of the isomers, and it is common to estimate other less commonly needed physical properties from a few measured key physical properties which can be easily measured, and which have been measured for 2,2,4,4-tetramethyl pentane.

The similarity to other hydrocarbons is also useful and is commonly used to predict unmeasured properties with good confidence.

The basic structure of n-nonane (normal nonane—the basic C\text{9} structure) is nine carbons in a row with all extra positions filled with hydrogen, as shown below:

\[
\begin{align*}
\text{CH}_3 & \quad (\text{CH}_2)\_7 \quad \text{CH}_3 \\
\text{n–nonane}
\end{align*}
\]

Other isomers of nonane include the three methyl isomers:

\[
\begin{align*}
\text{CH}_3 \\
\text{CH}_3 & \quad \text{CH} \quad (\text{CH}_2)\_5 \quad \text{CH}_3 \\
\text{2–methyl octane}
\end{align*}
\]
3-methyl octane

4-methyl octane

Note: 4-methyl octane would be the same as 3-methyl octane, but counting from the other end; thus, it is not named properly in the series. The rules minimize the numbers on the longest possible carbon chain.

This "isononane" series is followed by the dimethyl-heptane series, which is even more complicated because the two methyls can range from 2,2 to 3,4, with all nine of these possible:

2,2; 2,3; 2,4; 2,5; 2,6; 3,3; 3,4; 3,5; and 4,4; with higher counts just being mirror reflections of these counting from the higher (5) end.

The tri-methyl hexane series has the following eight isomers:

2,2,3; 2,2,4; 2,2,5; 2,3,3; 2,3,4; 2,3,5; 2,4,4 (=3,3,5); and 3,3,4;

and the tetra-methyl pentane series can have the four following isomers:

2,2,3,3; 2,2,3,4; 2,2,4,4 (the isomer under discussion); and 2,3,3,4.

In addition to the methyl isomers, ethyl isomers of nonane also exist. The first two isomers occur in the heptane sequence above as 3- or 4-ethyl heptane (2-ethyl heptane would be called 2-methyl octane). Shown below is 3-ethyl heptane.

The pentane base chain isomers of nonane include three dimethyl-ethyl isomers and one diethyl-pentane isomer (3,3-diethyl pentane, but the numbers are not required in this case), which can also be called tetra ethyl methane.

The three dimethyl ethyl isomers are 2,2-dimethyl, 3-ethyl pentane (also named isobutyl pentane); 2,3-dimethyl, 3-ethyl pentane (which can also be named 2-methyl, 3-isopropyl pentane in another naming system; this is the first of the isopropyl compounds to appear in the nonane isomer series); and 2,4-dimethyl, 3-ethyl pentane. Note that 2,2-dimethyl, 4-ethyl pentane would be named as a hexane.
The interesting thing about the 35 isomers of nonane is that most of them have very similar physical properties, and are very difficult to separate if mixed. Their chemical reactions also are similar enough that close isomers can be treated as if they were identical. Yet the difference between n-nonane and the complex nonane diagrammed immediately above in combustion in an engine is enough that n-nonane would be a good diesel fuel (igniting easily under compression) but a poor regular Otto cycle fuel (knocking badly, with a low octane number near zero) while the latter 2,2-dimethyl, 3-ethyl pentane would be a high-octane fuel for regular engines and a poor diesel fuel—just the opposite. Thus one must be careful about overgeneralizing similarities.

Table 1 shows some of the properties of the 35 isomers of nonane.

<table>
<thead>
<tr>
<th>ISOMER</th>
<th>BOILING POINT(°C)</th>
<th>MELTING POINT(°C)</th>
<th>DENSITY</th>
</tr>
</thead>
<tbody>
<tr>
<td>1  n-nonane</td>
<td>150.8</td>
<td>-51</td>
<td>0.7176</td>
</tr>
<tr>
<td>2  2-methyl octane</td>
<td>142.8</td>
<td>-80.1</td>
<td>0.7170</td>
</tr>
<tr>
<td>3  3-methyl octane</td>
<td>143</td>
<td>-107.6</td>
<td>0.7206</td>
</tr>
<tr>
<td>4  4-methyl octane</td>
<td>142.4</td>
<td>-113.2</td>
<td>0.7199</td>
</tr>
<tr>
<td>5  2,2-dimethyl heptane</td>
<td>132.7</td>
<td>-113</td>
<td>0.7105</td>
</tr>
<tr>
<td>6  2,3-dimethyl heptane</td>
<td>140.5</td>
<td>-116</td>
<td>0.7260</td>
</tr>
<tr>
<td>7  2,4-dimethyl heptane</td>
<td>133.5</td>
<td>-</td>
<td>0.7143</td>
</tr>
<tr>
<td>8  2,5-dimethyl heptane</td>
<td>136</td>
<td>-</td>
<td>0.7198</td>
</tr>
<tr>
<td>9  2,6-dimethyl heptane</td>
<td>135.2</td>
<td>-102.9</td>
<td>0.7989</td>
</tr>
<tr>
<td>10 3,3-dimethyl heptane</td>
<td>137.3</td>
<td>-</td>
<td>0.7254</td>
</tr>
<tr>
<td>11 3,4-dimethyl heptane</td>
<td>140.1</td>
<td>-</td>
<td>0.7314</td>
</tr>
<tr>
<td>12 3,5-dimethyl heptane</td>
<td>136</td>
<td>-</td>
<td>0.7225</td>
</tr>
<tr>
<td>13 4,4-dimethyl heptane</td>
<td>135.2</td>
<td>-</td>
<td>0.7221</td>
</tr>
<tr>
<td>14 3-ethyl heptane</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>15 4-ethyl heptane</td>
<td>141.2</td>
<td>-</td>
<td>0.7270</td>
</tr>
<tr>
<td>16 2,2,3-trimethyl hexane</td>
<td>131.7</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>17 2,2,4-trimethyl hexane</td>
<td>126.5</td>
<td>-120</td>
<td>0.711</td>
</tr>
<tr>
<td>18 2,2,5-trimethyl hexane</td>
<td>124</td>
<td>-105.8</td>
<td>0.7072</td>
</tr>
<tr>
<td>19 2,3,3-trimethyl hexane</td>
<td>137.7</td>
<td>-116.8</td>
<td>-</td>
</tr>
<tr>
<td>20 2,3,4-trimethyl hexane</td>
<td>139</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>21 2,3,5-trimethyl hexane</td>
<td>131.3</td>
<td>-127.9</td>
<td>0.7818</td>
</tr>
<tr>
<td>22 2,4,4-trimethyl hexane</td>
<td>126.5</td>
<td>-123.4</td>
<td>0.711</td>
</tr>
<tr>
<td>23 3,3,4-trimethyl hexane</td>
<td>140.5</td>
<td>-101.2</td>
<td>-</td>
</tr>
<tr>
<td>24 2,2,3,3-tetramethyl pentane</td>
<td>140.27</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>25 2,2,3,4-tetramethyl pentane</td>
<td>133.70</td>
<td>-</td>
<td>0.7389</td>
</tr>
<tr>
<td>26 2,2,4,4 (TMP under study)</td>
<td>122.7</td>
<td>-66.5</td>
<td>0.7195</td>
</tr>
<tr>
<td>27 2,3,3,4-tetramethyl pentane</td>
<td>141.5</td>
<td>-102.14</td>
<td>0.7547</td>
</tr>
<tr>
<td>28 2-methyl, 3-ethyl hexane</td>
<td>138</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>29 2-methyl, 4-ethyl hexane</td>
<td>133.8</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>30 3-methyl, 3-ethyl hexane</td>
<td>140.6</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>31 4-methyl, 3-ethyl hexane</td>
<td>140.4</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>32 2,2-dimethyl, 3-ethyl pentane</td>
<td>133.83</td>
<td>-99.7</td>
<td>0.74378</td>
</tr>
<tr>
<td>33 2,3-dimethyl, 3-ethyl pentane</td>
<td>141.6</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>34 2,4-dimethyl, 3-ethyl pentane</td>
<td>136.73</td>
<td>-122.4</td>
<td>0.7365</td>
</tr>
<tr>
<td>35 3,3-diethyl pentane</td>
<td>146.2</td>
<td>-33.1</td>
<td>0.7536</td>
</tr>
</tbody>
</table>
3.0 HAZARDS OF 2,2,4,4-TETRAMETHYL PENTANE (TMP) BY SIMILARITY TO OTHER NONANES, OCTANE, AND DECANE

Octane and decane are listed in the Handbook of Laboratory Safety, but neither nonane nor 2,2,4,4-tetramethyl pentane (TMP) is listed. Yet a very good estimate of the hazards of TMP may be formulated from the similarities of these compounds, since the nonanes lie between octane and decane.

The threshold limit value (TLV) of octane is 500 ppm (2350 mg/m³), with no limit listed for decane. We can probably consider 500 ppm as a conservative limit.

Octane and several other similar compounds suggest narcosis on inhalation exposure, and we probably should expect that with TMP.

Eye contact (3x). Minor residual injury expected in spite of prompt treatment from concentrated eye contact. Goggles required to prevent splash reaching eyes, safety glasses not quite sufficient.

Skin contact (2x). Minor residual injury from accidental exposure if prompt treatment is not given. We need to have facilities to wash off areas of contact promptly and be certain that those who may come in contact know that they must promptly remove TMP from skin.

Skin penetration (octane 1x, decane 3x, probable 2x). Exposure of 2 to 20 ml/kg body weight will give a lethal dose (LD) of LD-50. It is non-toxic in any reasonable quantity that would penetrate on short-term exposure. Prompt removal, as above, will preclude penetration through the skin.

Skin irritation (1x). No residual injury to skin from accidental exposure (causes only capillary injection).

Ingestion (1x). LD-50 for swallowing more than 10 gm/kg body weight. Avoid swallowing, but minor accidental ingestion not expected to be fatal; prompt medical treatment will be needed for major ingestion.

N.F.P.A. health hazard. 0, material which on exposure under fire conditions would offer no hazard beyond that of ordinary combustible material. Note that TMP is flammable (see next listing).

N.F.P.A. fire. Octane 3, decane 2. I recommend we conservatively treat TMP as 3, which is liquid that can be ignited under almost all ambient temperature conditions. (Liquids classified as "2" must be moderately heated before ignition.)

N.F.P.A. reactivity. 0, normally stable.

Extinguishing agents. 2,3 (foam and CO₂). Assume nitrogen or argon will also be effective.

Flammable limits. Octane, 1.0 to 4.66%; decane, 0.8 to 5.4%; thus we should expect about 0.9 to 5% flammable limits in air.

Flash point. Octane, 230°C; decane, 46°C. Pending better data we can treat TMP with the lower limit near 50°C and expect probable real flash point near 100°C (see boiling points). We should be conservative to be safe and treat it with lower limits until we have better data.

Ignition temperature. Octane, 230°C; decane, 208°C. Probable for TMP is about 220°C. We should alarm in space well below this value for other reasons, not a limiting factor.

Boiling point. Octane, 125°C; decane, 174.1°C. Known for TMP: 122.7°C.

Density. Octane, 0.7025; decane, 0.7300. Known for TMP: 0.7547.
REFERENCES
