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# ON DOMINATING SOMBOR ENERGY OF A GRAPH

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Abstract. In graph theory, a set of vertices $D \subseteq V(G)$ in a simple graph $G$ is termed a dominating set if every vertex not in $D$ is adjacent to at least one member of $D$, formally expressed as $N[D] = V(G)$. This work bridges these two concepts such as domination and topological indices. We establish several bounds for this new graph invariant. The paper concludes by demonstrating potential applications of new dominating energy in the field of chemistry.

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## 1. Introduction

All graphs considered in this paper are finite, simple and undirected. In particular, these graphs do not possess loops. Let $G = (V, E)$ be a graph with the vertex set $V(G) = \{v_1, v_2, v_3, \cdots, v_n\}$ and the edge set $E(G) = \{e_1, e_2, e_3, \cdots, e_m\}$, that is $|V(G)| = n$ and $|E(G)| = m$. The vertex $u$ and $v$ are adjacent if $uv \in E(G)$. The open(closed) neighborhood of a vertex $v \in V(G)$ is $N(v) = \{u : uv \in E(G)\}$ and $N[v] = N(v) \cup \{v\}$ respectively. The degree of a vertex $v \in V(G)$ is denoted by $d_G(v)$ and is defined as $d_G(v) = |N(v)|$. A vertex $v \in V(G)$ is pendant if $|N(v)| = 1$ and is called support vertex if it is adjacent to pendant vertex. Any vertex $v \in V(G)$ with $|N(v)| > 1$ is called internal vertex. If $d_G(v) = r$ for every vertex $v \in V(G)$, where $r \in \mathbb{Z}^+$ then $G$ is called r-regular. If $r = 2$ then it is called cycle graph $C_n$ and for $r = 3$ it is called the cubic graph. A graph $G$ is unicyclic If $|V| = |E|$. A graph $G$ is called a block graph, if every block in $G$ is a complete graph. For undefined terminologies we refer the reader to [15].

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Molecular descriptors give hope that the journey throughout endless chemical space won't be a random wandering but a methodical voyage toward substances of importance to mankind. Nowadays, there is a myriad of molecular descriptors, and among them, the topological indices have a prominent place. Topological index is simply a numeric associated with the molecular graph. So far, large number of such quantities are put forward by many researchers right from 1972[6]. An useful topological index is one which has a good predicting power in QSPR studies. Therefore, topological indices can be categorized into two categories useful and not so useful TI's. One of the most useful topological index is the Sombor index $SO(G)$ which is put forward by I Gutman[4]:

$$SO(G) = \sum_{uv \in E(G)} [\sqrt{deg(u)^2 + deg(v)^2}] \quad (1)$$

Boris Furtula and Ivan Gutman[2] have put forward a degree based topological indices viz., a forgotten topological index which is defined as

$$F(G) = \sum_{u \in V(G)} d_G(u)^3 = \sum_{uv \in E(G)} \left[d_G(u)^2 + d_G(v)^2\right].$$

A set $S \subseteq V$ is a *dominating set* of $G$ if each vertex in $V - S$ is adjacent to some vertex in $S$. The *domination number* $\gamma_{so}(G)$ is the smallest cardinality of a dominating set. A dominating set is said to be minimal, if no proper subset of $S$ is a dominating set of $G$. It is well known that, a maximal independent set of $G$ is a minimal dominating set of $G$. An excellent treatment of the fundamentals of domination is given in the book by Haynes et al. [9]. A survey of several advanced topics in domination is given in the book edited by Haynes et al. [10]. Various types of domination have been defined and studied by several authors and more than 75 models of domination are listed in the appendix of Haynes et al.[8].

The energy $E(G)$ of a graph $G$ is equal to the sum of the absolute values of the eigenvalues of the adjacency matrix of $G$. This quantity, introduced almost 30 years ago [12] and having a clear connection to chemical problems [14], has in newer times attracted much attention of mathematicians and mathematical chemists [8–11, 19, 21, 22, 26, 28].

In connection with energy (that is defined in terms of the eigenvalues of the adjacency matrix), energy-like quantities were considered also for the other matrices: Laplacian [14], distance [16], incidence [17], minimum covering energy [1] etc. Recall that a great variety of matrices has so far been associated with graphs [4, 5, 10, 27].

Motivated by Sombor index and domination number, here we define the minimum Sombor dominating matrix abbreviated as (S-dominating matrix). The S-dominating matrix of $G$ is the $n \times n$ matrix defined by $A_S(G) = (a_{ij})$, where

$$a_{ij} = \begin{cases} \sqrt{deg(v_i)^2 + deg(v_j)^2}, & \text{if } v_iv_j \in E; \\ 1, & \text{if } i = j \text{ and } v_i \in S; \\ 0, & \text{otherwise.} \end{cases}$$

The characteristic polynomial of $A_S(G)$ is denoted by $f_n(G, \lambda) := det(\lambda I - A_S(G))$.

The S-dominating eigenvalues of a graph $G$ are the eigenvalues of $A_S(G)$. Since $A_S(G)$ is real and symmetric, its eigenvalues are real numbers and we label them in non-increasing order $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. The S-dominating energy of $G$ is then defined as

$$E_S(G) = \sum_{i=1}^{n} |\lambda_i|.$$

**Note.** The Somber dominating matrix is similar to (but not identical with) the Sombor matrix of a graph with self-loops [2].

## 2. Results

We begin with the following straightforward observations. Note that the trace of $A_S(G) = \gamma(G)$.

Let $G = (V, E)$ be a graph with Sombor dominating set $S$. Let $f_n(G, \lambda) = c_0\lambda^n + c_1\lambda^{n-1} + \cdots + c_n$ be the characteristic polynomial of $A_S(G)$. Then

(1) $c_0 = 1$,
(2) $c_1 = -|D| = -\gamma_{so}(G)$.

**Theorem 2.1.** *If $\lambda_1, \lambda_2, \cdots, \lambda_n$ are the eigenvalues of $A_S(G)$, then*

$$\sum_{i=1}^{n} \lambda_i^2 \quad = \quad 2F(G) + \gamma_{so}(G).$$

We now obtain bounds for $E_S(G)$ of $G$, similar to McClelland's inequalities [20] for graph energy.

**Theorem 2.2.** *Let $G$ be a graph of order $n$ and size $m$ with $\gamma_{so}(G) = k$. Then*

$$E_S(G) \quad \leq \quad \sqrt{n(2m + k)}. \tag{2}$$

*Proof.* Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be the eigenvalues of $A_S(G)$. Bearing in mind the Cauchy-Schwarz inequality,

$$\left( \sum_{i=1}^{n} a_i b_i \right)^2 \leq \left( \sum_{i=1}^{n} a_i \right)^2 \left( \sum_{i=1}^{n} b_i \right)^2$$

we choose $a_i = 1$ and $b_i = |\lambda_i|$, which by Theorem 3 implies

$$E_S^2 \quad = \quad \left( \sum_{i=1}^{n} |\lambda_i| \right)^2$$

$$\begin{aligned} &\leq n\Big(\sum_{i=1}^{n}|\lambda_i|^2\Big)\\ &= n\sum_{i=1}^{n}\lambda_i^2\\ &= 2(2m+k). \end{aligned}$$

□

**Theorem 2.3.** *Let $G$ be a graph of order $n$ and size $m$ with $\gamma_{so}(G)=k$. Let $\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_n$ be a non-increasing arrangement of eigenvalues of $A_S(G)$. Then*

$$E_S(G) \geq \sqrt{2mn+nk-\alpha(n)(|\lambda_1|-|\lambda_n|)^2} \tag{3}$$

*where $\alpha(n)=n[\frac{n}{2}](1-\frac{1}{n}[\frac{n}{2}])$, where $[x]$ denotes the integer part of a real number $k$.*

*Proof.* Let $a_1,a_2,\cdots,a_n$ and $b_1,b_2,\cdots,b_n$ be real numbers for which there exist real constants $a,b,A$ and $B$, so that for each $i$, $i=1,2,\cdots,n, a\leq a_i\leq A$ and $b\leq b_i\leq B$. Then the following inequality is valid (see [6]).

$$|\, n\sum_{i=1}^{n}a_ib_i-\sum_{i=1}^{n}a_i\sum_{i=1}^{n}b_i\,| \leq \alpha(n)(A-a)(B-b) \tag{4}$$

where $\alpha(n)=n[\frac{n}{2}](1-\frac{1}{n}[\frac{n}{2}])$. Equality holds if and only if $a_1=a_2=\cdots=a_n$ and $b_1=b_2=\cdots=b_n$.
We choose $a_i:=|\lambda_i|, b_i:=|\lambda_i|$, $a=b:=|\lambda_n|$ and $A=B:=|\lambda_1|, i=1,2,\cdots,n$, inequality (4) becomes

$$|n\sum_{i=1}^{n}|\lambda_i|^2-\Big(\sum_{i=1}^{n}|\lambda_i|\Big)^2| \leq \alpha(n)(|\lambda_1|-|\lambda_n|)^2 \tag{5}$$

Since $E_{G_c}(G)=\sum\limits_{i=1}^{n}|\lambda_i|$, $\sum\limits_{i=1}^{n}|\lambda_i|^2=\sum\limits_{i=1}^{n}|\lambda_i|^2=2m+k$ and $E_S(G)\leq\sqrt{n(2m+k)}$, the inequality (5) becomes

$$\begin{aligned} n(2m+k)-(E_S)^2 &\leq \alpha(n)(|\lambda_1|-|\lambda_n|)^2\\ (E_S)^2 &\geq 2mn+nk-\alpha(n)(|\lambda_1|-|\lambda_n|)^2. \end{aligned}$$

Hence equality holds if and only if $\lambda_1=\lambda_2=\cdots=\lambda_n$. □

**Corollary 2.4.** *Let $G$ be a graph of order $n$ and size $m$ with $\gamma_{so}(G)=k$. Let $\lambda_1\geq\lambda_2\geq\cdots\geq\lambda_n$ be a non-increasing arrangement of eigenvalues of $A_S(G)$. Then*

$$E_S(G) \geq \sqrt{2mn+nk-\frac{n^2}{4}(|\lambda_1|-|\lambda_n|)^2} \tag{6}$$

*Proof.* Since $\alpha(n)=n[\frac{n}{2}](1-\frac{1}{n}[\frac{n}{2}])\leq\frac{n^2}{4}$, therefore by (3), result follows. □

**Theorem 2.5.** *Let $G$ be a graph of order $n$ and size $m$ with $\gamma_{so}(G) = k$. Let $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ be a non-increasing arrangement of eigenvalues of $A_S(G)$. Then*

$$E_{G_c}(G) \quad \geq \quad \frac{|\lambda_1||\lambda_2|n + 2m + k}{|\lambda_1| + |\lambda_n|} \tag{7}$$

*Proof.* Let $a_1, a_2, \cdots, a_n$ and $b_1, b_2, \cdots, b_n$ be real numbers for which there exist real constants $r$ and $R$ so that for each $i$, $i = 1, 2, \cdots, n$ holds $ra_i \leq b_i \leq Ra_i$. Then the following inequality is valid (see [11]).

$$\sum_{i=1}^{n} b_i^2 + rR\sum_{i=1}^{n} a_i^2 \quad \leq \quad (r+R)\sum_{i=1}^{n} a_i b_i. \tag{8}$$

Equality of (8) holds if and only if, for at least one $i$, $1 \leq i \leq n$ holds $ra_i = b_i = Ra_i$.
For $b_i := |\lambda_i|$, $a_i := 1$ $r := |\lambda_n|$ and $R := |\lambda_1|$, $i = 1, 2, \cdots, n$ inequality (8) becomes

$$\sum_{i=n}^{n} |\lambda_i|^2 + |\lambda_1||\lambda_n| \sum_{i=1}^{n} 1 \leq (|\lambda_1| + |\lambda_n|) \sum_{i=1}^{n} |\lambda_i|. \tag{9}$$

Since $\sum\limits_{i=1}^{n} |\lambda_i|^2 = \sum\limits_{i=1}^{n} \lambda_i^2 = 2m + k$, $\sum\limits_{i=1}^{n} |\lambda_i| = E_S(G)$, from inequality (9),

$$2m + k + |\lambda_1||\lambda_n|n \quad \leq \quad (\lambda_1 + \lambda_n)E_S(G)$$

Hence the result. □

**Theorem 2.6.** *Let $G$ be a graph of order $n$ and size $m$ with $\gamma_{so}(G) = k$. If $\xi = |detA_S(G)|$, then*

$$E_S(G) \quad \geq \quad \sqrt{2m + k + n(n-1)\xi^{\frac{2}{n}}}. \tag{10}$$

*Proof.*

$$\begin{aligned}(E_S(G))^2 \quad &= \quad \left(\sum_{i=1}^{n} |\lambda_i|\right)^2 \\ &= \quad \sum_{i=1}^{n} |\lambda_i|^2 + \sum_{i \neq j} |\lambda_i||\lambda_j|.\end{aligned}$$

Employing the inequality between the arithmetic and geometric means, we obtain

$$\frac{1}{n(n-1)} \sum_{i \neq j} |\lambda_i||\lambda_j| \quad \geq \quad \left(\prod_{i \neq j} |\lambda_i||\lambda_j|\right)^{\frac{1}{n(n-1)}}.$$

Thus,

$$(E_{D_G})^2 \quad \geq \quad \sum_{i=1}^{n} |\lambda_i|^2 + n(n-1)\left(\prod_{i \neq j} |\lambda_i||\lambda_j|\right)^{\frac{1}{n(n-1)}}$$

$$\begin{aligned} &\geq \sum_{i=1}^{n} |\lambda_i|^2 + n(n-1)\Big(\prod_{i\neq j} |\lambda_i|^{2(n-1)}\Big)^{\frac{1}{n(n-1)}} \\ &= 2m + k + n(n-1)\xi^{\frac{2}{n}} \end{aligned}$$

□

**Lemma 2.7.** *If $\lambda_1(G)$ is the largest minimum connected dominating eigenvalue of $A_S(G)$, then $\lambda_1 \geq \frac{2m+\gamma_{so}(G)}{n}$.*

*Proof.* Let $X$ be any non-zero vector. Then we have $\lambda_1(A) = max_{X\neq 0}\{\frac{X'AX}{X'X}\}$, see [15]. Therefore, $\lambda_1(A_S(G)) \geq \frac{J'AJ}{J'J} = \frac{2m+\gamma_{so}(G)}{n}$. □

Next, we obtain Koolen and Moulton's [18] type inequality for $E_S(G)$.

**Theorem 2.8.** *If $G$ is a graph of order $n$ and size $m$ and $2m + \gamma_C(G) \geq n$, then*

$$E_S(G) \leq \frac{2m+\gamma_{so}(G)}{n} + \sqrt{(n-1)\Big[(2m+\gamma_{so}(G)) - \Big(\frac{2m+\gamma_{so}(G)}{n}\Big)^2\Big]} \quad (11)$$

*Proof.* Bearing in mind the Cauchy-Schwarz inequality,

$$\Big(\sum_{i=1}^{n} a_i b_i\Big)^2 \leq \Big(\sum_{i=1}^{n} a_i\Big)^2 \Big(\sum_{i=1}^{n} b_i\Big)^2.$$

Put $a_i = 1$ and $b_i = |\lambda_i|$ then

$$\begin{aligned} \Big(\sum_{i=2}^{n} a_i b_i\Big)^2 &\leq (n-1)\Big(\sum_{i=2}^{n} b_i\Big)^2 \\ (E_S(G) - \lambda_1)^2 &\leq (n-1)(2m + \gamma_{so}(G) - \lambda_1^2) \\ E_S(G) &\leq \lambda_1 + \sqrt{(n-1)(2m + \gamma_{so}(G) - \lambda_1^2)}. \end{aligned}$$

Let

$$f(x) = x + \sqrt{(n-1)(2m + \gamma_{so}(G) - x^2)} \quad (12)$$

For decreasing function

$$\begin{aligned} f'(x) &\leq 0 \\ \Rightarrow 1 - \frac{x(n-1)}{\sqrt{(n-1)(2m+\gamma_{so}(G) - x^2)}} &\leq 0 \\ x &\geq \sqrt{\frac{2m+\gamma_{so}(G)}{n}}. \end{aligned}$$

Since $(2m + k) \geq n$, we have $\sqrt{\frac{2m+\gamma_{so}(G)}{n}} \leq \frac{2m+\gamma_{so}(G)}{n} \leq \lambda_1$. Also $f(\lambda_1) \leq f\Big(\frac{2m+\gamma_{so}(G)}{n}\Big)$.

$$\text{i.e } E_S(G) \leq f(\lambda_1) \leq f\left(\frac{2m+\gamma_{so}(G)}{n}\right).$$

$$\text{i.e } E_S(G) \leq f\left(\frac{2m+\gamma_{so}(G)}{n}\right)$$

Hence by (12), the result follows. □

## 3. Chemical Applicability of $E_S(G)$

The boiling point of compound is an important physical property for the design and optimization of the processing engineering in chemical and petrochemical industries. Therefore it is important to develop quantitative structure boiling point models for the estimation of boiling points of untested compounds or selection of reliable experimental boiling points of the compounds. Oxo indicates a double bond between an oxygen and carbon atoms. Oxo chemicals are intermediate and derivative chemical compounds which are characteristically used in chemical and manufacturing processes of paints, plasticizers, coatings, adhesives and lubricant additives.

**Data Set**

There are 192 oxo chemicals in the data collection, comprising 32 aldehydes, 78 ethers, and 82 ketons (Table 1). Ref[4] is where the calculated and experimental

boiling points are found. Table 2 also contains values of molecular descriptors of 192 oxo compounds.

| Sl. No. | Compound Name | Exp | Calcd | GNI | SLI | MSLI | FSLI | MFSLI | SCGI | PCGI | MASCI | SAI | RSI |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | Dimethyl ether | -24.9 | -24 | 4.47 | 4.47 | 0.89 | 8.24 | 0.48 | 0.89 | 0.81 | 0.33 | 54.0 | 5.00 |
| 2 | Ethyl methyl ether | 7.4 | 8.3 | 7.3 | 7.3 | 1.24 | 13.9 | 0.66 | 1.24 | 1.06 | 0.23 | 62 | 7.07 |
| 3 | Methyl propyl ether | 38.6 | 39.3 | 10.12 | 10.12 | 1.6 | 19.55 | 0.83 | 1.6 | 1.31 | 0.16 | 70 | 10 |
| 4 | Diethyl ether | 34.6 | 37.1 | 10.12 | 10.12 | 1.6 | 19.55 | 0.83 | 1.6 | 1.31 | 0.16 | 70 | 10 |
| 5 | Isopropyl methyl ether | 30.8 | 30.1 | 10.84 | 12.16 | 1.35 | 32.08 | 0.56 | 1.5 | 1.16 | 0.22 | 47.62 | 80.62 |
| 6 | Butyl methyl ether | 70.3 | 68.9 | 12.95 | 12.95 | 1.95 | 25.21 | 1.01 | 1.95 | 1.56 | 0.11 | 78 | 14.14 |
| 7 | Ethyl propyl ether | 63.9 | 65.3 | 12.95 | 12.95 | 1.95 | 25.21 | 1.01 | 1.95 | 1.56 | 0.11 | 78 | 14.14 |
| 8 | Ethyl isopropyl ether | 54.1 | 56.5 | 13.67 | 14.99 | 1.71 | 37.73 | 0.74 | 1.85 | 1.41 | 0.15 | 55.62 | 228.03 |
| 9 | Isobutyl methyl ether | 58.6 | 60.2 | 13.67 | 14.99 | 1.71 | 37.73 | 0.74 | 1.85 | 1.41 | 0.15 | 55.62 | 228.03 |
| 10 | Sec-butyl methyl ether | 59 | 57.5 | 13.75 | 14.84 | 1.76 | 36.99 | 0.79 | 1.87 | 1.47 | 0.14 | 71.25 | 205.54 |
| 11 | Tert-butyl methyl ether | 52 | 50.9 | 14.97 | 19.07 | 1.39 | 68.7 | 0.49 | 1.71 | 1.22 | 0.21 | 44.26 | 1108.26 |
| 12 | Methyl pentyl ether | 99 | 97.3 | 15.78 | 15.78 | 2.3 | 30.87 | 1.19 | 2.3 | 1.81 | 0.08 | 86 | 20 |
| 13 | Ethyl butyl ether | 92.2 | 92.6 | 15.78 | 15.78 | 2.3 | 30.87 | 1.19 | 2.3 | 1.81 | 0.08 | 86 | 20 |
| 14 | Dipropyl ether | 89.6 | 91.2 | 15.78 | 15.78 | 2.3 | 30.87 | 1.19 | 2.3 | 1.81 | 0.08 | 86 | 20 |
| 15 | Isopropyl propyl ether | 83 | 82.5 | 16.5 | 17.82 | 2.06 | 29.33 | 1.25 | 2.21 | 1.66 | 0.11 | 63.62 | 644.98 |
| 16 | Ethyl isobutyl ether | 82 | 83.9 | 16.5 | 17.82 | 2.06 | 29.33 | 1.25 | 2.21 | 1.66 | 0.11 | 63.62 | 644.98 |
| 17 | Isopentyl methyl ether | 91 | 88.7 | 16.5 | 17.82 | 2.06 | 29.33 | 1.25 | 2.21 | 1.66 | 0.11 | 63.62 | 644.98 |
| 18 | Methyl 1-methylbutyl ether | 91.5 | 84.8 | 16.57 | 17.67 | 2.11 | 42.65 | 0.97 | 2.22 | 1.72 | 0.1 | 79.25 | 581.37 |
| 19 | Methyl 2-methylbutyl ether | 93 | 86.6 | 16.57 | 17.67 | 2.11 | 42.65 | 0.97 | 2.22 | 1.72 | 0.1 | 79.25 | 581.37 |
| 20 | Diisopropyl ether | 69 | 73.6 | 17.21 | 19.86 | 1.81 | 55.91 | 0.64 | 2.11 | 1.51 | 0.15 | 41.25 | 500 |
| 21 | Methyl tert-pentyl ether | 86.3 | 76.1 | 17.95 | 82.66 | 1.82 | 73.29 | 0.73 | 2.09 | 1.55 | 0.13 | 70 | 4250 |
| 22 | 1,2-dimethylpropyl methyl ether | 81.3 | 76.3 | 17.36 | 19.57 | 1.9 | 53.86 | 0.75 | 2.14 | 1.59 | 0.12 | 59 | 360.55 |
| 23 | 2,2-dimethylpropyl methyl ether | 80.5 | 80.9 | 17.8 | 21.9 | 1.75 | 74.36 | 0.66 | 2.06 | 1.47 | 0.15 | 52.26 | 4701.96 |
| 24 | 1-ethylpropyl methyl ether | 88.5 | 81.9 | 16.65 | 17.52 | 2.17 | 41.91 | 1.03 | 2.24 | 1.77 | 0.08 | 94.88 | 524.04 |
| 25 | Ethyl tert-butyl ether | 73.1 | 76 | 17.8 | 21.9 | 1.75 | 74.36 | 0.66 | 2.06 | 1.47 | 0.15 | 52.26 | 4701.96 |
| 26 | Hexyl methyl ether | 125 | 124.5 | 18.61 | 18.61 | 2.66 | 36.53 | 1.36 | 2.66 | 2.06 | 0.05 | 94 | 28.28 |
| 27 | Ethyl propyl ether | 118 | 118.8 | 12.95 | 12.95 | 1.95 | 25.21 | 1.01 | 1.95 | 1.56 | 0.11 | 78 | 14.14 |
| 28 | Butyl propyl ether | 117.1 | 116.4 | 18.61 | 18.61 | 2.66 | 36.53 | 1.36 | 2.66 | 2.06 | 0.05 | 94 | 28.28 |
| 29 | Butyl isopropyl ether | 107 | 107.6 | 19.32 | 20.65 | 2.41 | 49.05 | 1.09 | 2.56 | 1.91 | 0.07 | 71.62 | 1824.28 |
| 30 | Isobutyl propyl ether | 106 | 107.6 | 19.32 | 20.65 | 2.41 | 49.05 | 1.09 | 2.56 | 1.91 | 0.07 | 71.62 | 1824.28 |
| 31 | Ethyl isopentyl ether | 111 | 110 | 19.32 | 20.65 | 2.41 | 49.05 | 1.09 | 2.56 | 1.91 | 0.07 | 71.62 | 1824.28 |
| 32 | Tert-butyl propyl ether | 100 | 100.9 | 20.63 | 24.73 | 2.1 | 80.02 | 0.84 | 2.42 | 1.72 | 0.1 | 60.26 | 19948.75 |
| 33 | Tert-isobutyl propyl ether | 87.6 | 91.8 | 21.34 | 26.77 | 1.86 | 92.54 | 0.57 | 2.32 | 1.57 | 0.14 | 37.89 | 15983.61 |
| 34 | Ethyl 1-ethylbutyl ether | 105.5 | 103.8 | 19.4 | 20.5 | 2.47 | 48.31 | 1.15 | 2.58 | 1.97 | 0.07 | 87.25 | 1644.38 |
| 35 | 2,2-dimethylpropyl ethyl ether | 91.5 | 103.4 | 20.63 | 24.73 | 2.1 | 80.02 | 0.84 | 2.42 | 1.72 | 0.109 | 60.26 | 19948.75 |
| 36 | Ethyl 2-ethyl butyl ether | 109.5 | 104.4 | 16.5 | 17.82 | 2.06 | 29.33 | 1.25 | 2.21 | 1.66 | 0.11 | 63.62 | 644.98 |
| 37 | Ethyl tert-pentyl ether | 101 | 99.4 | 17.95 | 21.66 | 1.82 | 73.29 | 0.73 | 2.09 | 1.55 | 0.13 | 70 | 4250 |
| 38 | 1,2-dimethylpropyl ethyl ether | 99.3 | 102.3 | 20.19 | 22.39 | 2.26 | 59.52 | 0.93 | 2.49 | 1.84 | 0.09 | 67 | 1019.8 |
| 39 | Dibutyl ether | 140.3 | 139.8 | 21.44 | 21.44 | 3.01 | 42.18 | 1.54 | 3.01 | 2.31 | 0.04 | 102 | 40 |
| 40 | Isopentyl propyl ether | 125 | 131.6 | 22.15 | 23.47 | 2.77 | 54.71 | 1.27 | 2.91 | 2.16 | 0.05 | 79.62 | 5159.84 |
| 41 | Butyl isobutyl ether | 132 | 130.6 | 19.32 | 20.65 | 2.41 | 49.05 | 1.09 | 2.56 | 1.91 | 0.07 | 71.62 | 1824.28 |
| 42 | Butyl sec-butyl ether | 130.5 | 129.8 | 22.23 | 23.33 | 2.82 | 53.96 | 1.32 | 2.93 | 2.22 | 0.05 | 95.25 | 4651.02 |
| 43 | Butyl tert-butyl ether | 125 | 124.9 | 23.46 | 27.56 | 2.45 | 85.67 | 1.02 | 2.77 | 1.97 | 0.07 | 68.26 | 84635.41 |
| 44 | Sec-butyl isobutyl ether | 122 | 120.6 | 22.95 | 25.36 | 2.58 | 66.49 | 1.05 | 2.83 | 2.07 | 0.06 | 72.88 | 3605.55 |
| 45 | di-sec-butyl ether | 121 | 119.7 | 23.03 | 25.21 | 2.63 | 65.75 | 1.11 | 2.85 | 2.12 | 0.06 | 88.51 | 3250 |
| 46 | Diisobutyl ether | 122.2 | 121.3 | 22.87 | 25.51 | 2.52 | 67.23 | 0.99 | 2.82 | 2.01 | 0.07 | 57.25 | 4000 |
| 47 | Isobutyl tert-butyl ether | 111.5 | 115.5 | 24.17 | 29.59 | 2.21 | 98.2 | 0.74 | 2.67 | 1.81 | 0.1 | 45.89 | 67812.75 |
| 48 | di-tert-butyl ether | 107.3 | 109 | 25.48 | 33.68 | 1.9 | 129.17 | 0.49 | 2.53 | 1.63 | 0.14 | 34052 | 49130 |
| 49 | Isopropyl tert-pentyl ether | 114.5 | 113.7 | 24.32 | 29.35 | 2.28 | 97.13 | 0.81 | 2.7 | 1.9 | 0.08 | 63.63 | 61294.37 |
| 50 | Hexyl ethyl ether | 143 | 114 | 21.44 | 21.44 | 3.01 | 42.18 | 1.54 | 3.01 | 2.31 | 0.041 | 102 | 40 |
| 51 | Heptyl methyl ether | 151 | 150.5 | 21.44 | 21.44 | 3.01 | 42.18 | 1.54 | 3.01 | 2.31 | 0.041 | 102 | 40 |
| 52 | 1-ethylpropyl propyl ether | 128.5 | 126.5 | 19.4 | 20.5 | 2.47 | 48.31 | 1.15 | 2.58 | 1.97 | 0.07 | 87.25 | 1655.38 |
| 53 | Ethyl 1-methylpentyl ether | 125 | 131.9 | 22.23 | 23.33 | 2.82 | 53.96 | 1.32 | 2.93 | 2.22 | 0.05 | 95.25 | 4651.02 |
| 54 | Ethyl heptyl ether | 166.6 | 168.3 | 24.27 | 24.27 | 3.36 | 47.84 | 1.72 | 3.36 | 2.56 | 0.02 | 110 | 56.56 |
| 55 | Butyl isopentyl ether | 157 | 152.8 | 24.98 | 26.3 | 3.12 | 60.36 | 1.44 | 3.27 | 2.41 | 0.03 | 87.62 | 14594.24 |
| 56 | Tert-butyl isopentyl ether | 139 | 137.9 | 27 | 32.42 | 2.56 | 103.85 | 0.92 | 3.03 | 2.07 | 0.07 | 53.89 | 287705.09 |
| 57 | Butyl pentyl ether | 163 | 162.5 | 24.27 | 24.27 | 3.36 | 47.84 | 1.72 | 3.36 | 2.56 | 0.02 | 110 | 56.56 |
| 58 | Isopropyl isopentyl ether | 139 | 143.7 | 22.87 | 25.51 | 2.52 | 67.23 | 0.99 | 2.82 | 2.01 | 0.07 | 57.25 | 4000 |
| 59 | Methyl 1-methylheptyl ether | 162 | 160.7 | 25.06 | 26.15 | 3.17 | 59.62 | 1.5 | 3.28 | 2.47 | 0.03 | 103.25 | 13155.07 |
| 60 | Methyl octyl ether | 173 | 175.4 | 24.27 | 24.27 | 3.36 | 47.84 | 1.72 | 3.36 | 2.56 | 0.02 | 110 | 56.56 |
| 61 | 3,5-dimethylhexyl methyl ether | 155.5 | 155.2 | 25.78 | 28.19 | 2.93 | 72.14 | 1.23 | 3.19 | 2.32 | 0.04 | 80.88 | 10198.03 |
| 62 | Ethyl octyl ether | 189.2 | 191.6 | 3.72 | 2.81 | 0.02 | 53.5 | 1.89 | 3.72 | 2.81 | 0.02 | 118 | 80 |
| 63 | Ethyl 1,1,3,3-tetramethylbutyl ether | 156.5 | 155.4 | 28.46 | 36.26 | 2.33 | 133.75 | 0.73 | 2.91 | 1.95 | 0.08 | 60.27 | 188404.94 |
| 64 | bis(1-ethylpropyl) ether | 161.5 | 159.1 | 25.93 | 27.89 | 3.04 | 70.66 | 1.34 | 3.22 | 2.42 | 0.03 | 112.14 | 8285.9 |
| 65 | bis(1-methylbutyl) ether | 162 | 163.3 | 28.68 | 30.87 | 3.34 | 77.06 | 1.46 | 3.56 | 2.62 | 0.03 | 104.51 | 26000 |
| 66 | Butyl 1-methylpentyl ether | 170 | 173.7 | 27.89 | 28.98 | 3.53 | 65.28 | 1.68 | 3.64 | 2.72 | 0.02 | 111.25 | 37208.17 |
| 67 | diisopentyl ether | 172 | 163 | 28.52 | 31.17 | 3.23 | 78.54 | 1.35 | 3.52 | 2.51 | 0.03 | 73.25 | 32000 |
| 68 | dipentyl ether | 186.8 | 183.6 | 3.72 | 2.81 | 0.02 | 53.5 | 1.89 | 3.72 | 2.81 | 0.02 | 118 | 80 |
| 69 | Isopropyl heptyl ether | 173 | 176.7 | 27.81 | 29.13 | 3.47 | 66.02 | 1.62 | 3.62 | 2.66 | 0.02 | 95.62 | 41278.75 |
| 70 | heptyl propyl ether | 187 | 186.9 | 3.72 | 2.81 | 0.02 | 53.5 | 1.89 | 3.72 | 2.81 | 0.02 | 118 | 80 |
| 71 | Isopentyl pentyl ether | 174 | 173.3 | 27.81 | 29.13 | 3.47 | 66.02 | 1.62 | 3.62 | 2.66 | 0.02 | 95.62 | 41278.75 |
| 72 | methyl 1-methyloctyl ether | 188.5 | 183.8 | 27.89 | 28.98 | 3.53 | 65.28 | 1.68 | 3.64 | 2.72 | 0.02 | 111.25 | 37208.17 |
| 73 | octyl propyl ether | 204 | 208.8 | 29.92 | 29.92 | 4.07 | 59.15 | 2.07 | 4.07 | 3.06 | 0.01 | 126 | 113.13 |
| 74 | Isopropyl octyl ether | 198.5 | 197.8 | 30.64 | 31.96 | 3.83 | 71.68 | 1.8 | 3.97 | 2.91 | 0.01 | 103.62 | 116753.96 |
| 75 | dihexyl ether | 225.7 | 223.3 | 33.34 | 33.34 | 4.33 | 64.81 | 2.25 | 4.33 | 3.15 | 0.01 | 115 | 101.19 |

| Sl. No. | Compound Name | Exp | Calcd | GNI | SLI | MSLI | FSLI | MFSLI | SCGI | PCGI | MASCI | SAI | RSI |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 76 | diheptyl ether | 258.5 | 259.2 | 38.41 | 38.41 | 5.13 | 76.12 | 2.6 | 5.13 | 3.81 | 0.005 | 150 | 320 |
| 77 | dioctyl ether | 291.7 | 291.6 | 44.07 | 44.07 | 5.84 | 87.44 | 2.95 | 5.84 | 4.31 | 0.002 | 166 | 640 |
| 78 | bis(2-ethylhexyl) ether | 269.8 | 268.2 | 45.81 | 47.54 | 5.57 | 109.52 | 2.64 | 5.71 | 4.22 | 0.003 | 183.77 | 10816000 |
| 79 | acetaldehyde | 20.8 | 19. | 4.47 | 4.47 | 0.89 | 8.24 | 0.48 | 0.89 | 0.81 | 0.33 | 54 | 5 |
| 80 | propionaldehyde | 48.8 | 50.6 | 7.3 | 7.3 | 1.24 | 13.9 | 0.66 | 1.24 | 1.06 | 0.23 | 62 | 7.07 |
| 81 | butyl aldehyde | 75.7 | 78.5 | 10.12 | 10.12 | 1.6 | 19.55 | 0.83 | 1.6 | 1.31 | 0.16 | 70 | 10 |
| 82 | pentaldehyde | 103 | 104.5 | 12.95 | 12.95 | 1.95 | 25.21 | 1.01 | 1.95 | 1.56 | 0.11 | 78 | 14.14 |
| 83 | 2-methyl butanal | 92.5 | 95.8 | 13.75 | 14.84 | 1.76 | 36.99 | 0.79 | 1.87 | 1.47 | 0.14 | 71.25 | 205.54 |
| 84 | 3-methyl butanal | 92.5 | 97.1 | 13.67 | 14.99 | 1.71 | 37.73 | 0.74 | 1.85 | 1.41 | 0.15 | 55.62 | 228.03 |
| 85 | 2,2-dimethyl propanal | 77.5 | 79 | 14.97 | 19.07 | 1.39 | 68.7 | 0.49 | 1.71 | 1.22 | 0.21 | 44.26 | 1108.26 |
| 86 | Hexanal | 128 | 128.9 | 15.78 | 15.78 | 2.3 | 30.87 | 1.19 | 2.3 | 1.81 | 0.08 | 86 | 20 |
| 87 | 2-methylpentanal | 117 | 119.6 | 16.57 | 17.67 | 2.11 | 42.65 | 0.97 | 2.22 | 1.72 | 0.1 | 79.25 | 581.37 |
| 88 | 3-methylpentanal | 118 | 120.6 | 16.57 | 17.67 | 2.11 | 42.65 | 0.97 | 2.22 | 1.72 | 0.1 | 79.25 | 581.37 |
| 89 | 4-methylpentanal | 121 | 121.6 | 16.5 | 17.82 | 2.06 | 43.39 | 0.91 | 2.21 | 1.66 | 0.11 | 63.62 | 644.98 |
| 90 | 2-ethylbutaanal | 117 | 117.7 | 16.65 | 17.52 | 2.17 | 41.91 | 1.03 | 2.24 | 1.77 | 0.08 | 94.88 | 524.04 |
| 91 | heptanal | 152.8 | 151.8 | 18.61 | 18.61 | 2.66 | 36.53 | 1.36 | 2.66 | 2.06 | 0.05 | 94 | 28.28 |
| 92 | 2-methyl hexanal | 141 | 142.3 | 19.4 | 20.5 | 2.47 | 48.31 | 1.15 | 2.58 | 1.97 | 0.07 | 87.25 | 1644.38 |
| 93 | 3-methyl hexanal | 143 | 143 | 16.57 | 17.67 | 2.11 | 42.65 | 0.97 | 2.22 | 1.72 | 0.1 | 79.25 | 581.37 |
| 94 | 4-methyl hexanal | 144 | 143.7 | 19.4 | 20.5 | 2.47 | 48.31 | 1.15 | 2.58 | 1.97 | 0.07 | 87.25 | 1644.38 |
| 95 | 5-methyl hexanal | 143.5 | 144.2 | 19.32 | 20.65 | 2.41 | 49.05 | 1.09 | 2.56 | 1.91 | 0.07 | 71.62 | 1824.28 |
| 96 | 2,2-dimethylpentanal | 126.5 | 131.8 | 20.78 | 24.49 | 2.18 | 78.95 | 0.9 | 2.44 | 1.8 | 0.09 | 78.009 | 18031.22 |
| 97 | 2,3-dimethylpentanal | 141 | 134.1 | 20.26 | 22.25 | 2.31 | 58.78 | 0.98 | 2.51 | 1.89 | 0.08 | 82.63 | 919.23 |
| 98 | octanal | 171 | 176.6 | 21.44 | 21.44 | 3.01 | 42.18 | 1.54 | 3.01 | 2.31 | 0.04 | 102 | 40 |
| 99 | 2-ethylhexanal | 160 | 161.1 | 22.31 | 23.18 | 2.88 | 53.22 | 1.38 | 2.95 | 2.27 | 0.04 | 110.88 | 4192.37 |
| 100 | 2-propylpentanal | 160 | 160.2 | 22.31 | 23.18 | 2.88 | 53.22 | 1.38 | 2.95 | 2.27 | 0.04 | 110.88 | 4192.37 |
| 101 | nonanal | 191 | 194.2 | 24.27 | 14.27 | 3.36 | 47.84 | 1.72 | 3.36 | 2.56 | 0.02 | 110 | 56.56 |
| 102 | 3,5,5-trimethyl hexanal | 170.5 | 166.7 | 27.08 | 32.27 | 2.62 | 103.11 | 0.98 | 3.04 | 2.12 | 0.06 | 69.52 | 273361.9 |
| 103 | decanal | 208.5 | 213.9 | 27.09 | 27.09 | 3.72 | 53.5 | 1.89 | 3.72 | 2.81 | 0.02 | 118 | 82 |
| 104 | undecanal | 233 | 232.7 | 29.92 | 29.92 | 4.07 | 59.15 | 2.07 | 4.07 | 3.06 | 0.01 | 126 | 113.13 |
| 105 | 2-methyl decanal | 229 | 221.7 | 30.72 | 31.81 | 3.88 | 70.94 | 1.85 | 3.99 | 2.97 | 0.01 | 119.25 | 105240.6 |
| 106 | dodecanal | 254 | 250.6 | 32.75 | 32.75 | 4.42 | 64.81 | 2.25 | 4.42 | 3.31 | 0.01 | 134 | 425984 |
| 107 | 2-methylundecanal | 246 | 239 | 33.55 | 34.64 | 4.24 | 76.59 | 2.03 | 4.35 | 3.22 | 0.01 | 127.25 | 297665.36 |
| 108 | tridecanal | 267 | 267.8 | 35.58 | 35.58 | 4.78 | 70.47 | 2.42 | 4.78 | 3.56 | 0.007 | 142 | 226.27 |
| 109 | tetradecanal | 287 | 284.2 | 38.41 | 38.41 | 5.13 | 76.12 | 2.6 | 5.13 | 3.81 | 0.005 | 150 | 320 |
| 110 | pentadecanal | 304.9 | 299.9 | 41.24 | 41.24 | 5.49 | 81.78 | 2.78 | 5.49 | 4.06 | 0.003 | 158 | 452.54 |
| 111 | acetone | 56.2 | 47.4 | 7.93 | 9.48 | 0.94 | 27.16 | 0.33 | 1.13 | 0.86 | 0.35 | 24 | 31.62 |
| 112 | 2-butanone | 79.6 | 75.4 | 10.84 | 12.16 | 1.35 | 32.08 | 0.56 | 1.5 | 1.16 | 0.22 | 47.62 | 80.62 |
| 113 | 2-pentanone | 102 | 100.4 | 13.67 | 14.99 | 1.71 | 37.73 | 0.74 | 1.85 | 1.41 | 0.15 | 55.62 | 228.03 |
| 114 | 3-pentanone | 101.7 | 98.3 | 13.75 | 14.84 | 1.76 | 36.99 | 0.79 | 1.87 | 1.47 | 0.14 | 71.25 | 205.54 |
| 115 | 3-methyl-2-butanone | 93.5 | 92.7 | 14.45 | 16.89 | 1.5 | 48.94 | 0.52 | 1.77 | 1.29 | 0.2 | 35.375 | 141.42 |
| 116 | 2-hexanone | 127 | 125.2 | 16.5 | 17.82 | 2.06 | 43.39 | 0.91 | 2.21 | 1.66 | 0.11 | 63.62 | 644.98 |
| 117 | 3-hexanone | 123.5 | 122.2 | 16.57 | 17.67 | 2.11 | 42.65 | 0.97 | 2.22 | 1.72 | 0.1 | 79.25 | 581.37 |
| 118 | 3-methyl-2-pentanone | 118 | 116 | 13.67 | 14.99 | 1.71 | 37.73 | 0.74 | 1.85 | 1.41 | 0.15 | 55.62 | 228.03 |
| 119 | 4-metyl-2-pentanone | 117 | 117.4 | 17.21 | 19.86 | 1.81 | 55.91 | 0.64 | 2.11 | 1.51 | 0.15 | 41.25 | 500 |
| 120 | 2-methyl-3-pentanone | 115.5 | 114.5 | 17.36 | 19.57 | 1.9 | 53.86 | 0.75 | 2.14 | 1.59 | 0.12 | 59.004 | 360.55 |
| 121 | 3,3-dimethyl-2-butanone | 106 | 107.3 | 18.65 | 23.69 | 1.56 | 84.56 | 0.46 | 1.98 | 1.35 | 0.19 | 32.63 | 3134.64 |
| 122 | 2-heptanone | 151.4 | 148.5 | 19.32 | 20.65 | 2.41 | 49.05 | 1.09 | 2.56 | 1.91 | 0.07 | 71.62 | 1824.28 |
| 123 | 3-heptanone | 147 | 145.4 | 17.4 | 20.5 | 2.47 | 48.31 | 1.15 | 2.58 | 1.97 | 0.07 | 87.25 | 1644.38 |
| 124 | 4-heptanone | 144 | 144.4 | 19.4 | 20.5 | 2.47 | 48.31 | 1.15 | 2.58 | 1.97 | 0.07 | 87.25 | 1644.38 |
| 125 | 3-methyl-2-hexanone | 143.5 | 139.5 | 20.19 | 22.39 | 2.26 | 59.52 | 0.93 | 2.49 | 1.84 | 0.09 | 67.004 | 1019.8 |
| 126 | 4-methyl-2-hexanone | 139 | 139.7 | 20.12 | 22.53 | 2.22 | 60.83 | 0.87 | 2.48 | 1.82 | 0.09 | 64.88 | 1274.75 |
| 127 | 5-methyl-2-hexanone | 144 | 140.5 | 20.04 | 22.68 | 2.17 | 61.57 | 0.82 | 2.46 | 1.76 | 0.1 | 49.25 | 1414.21 |
| 128 | 2-methyl-3-hexanone | 135 | 134.2 | 20.19 | 22.39 | 2.26 | 59.52 | 0.93 | 2.49 | 1.84 | 0.09 | 67.004 | 1019.8 |
| 129 | 4-methyl-3-hexanone | 134.5 | 136.4 | 20.26 | 22.25 | 2.31 | 58.78 | 0.98 | 2.51 | 1.89 | 0.08 | 82.63 | 919.23 |
| 130 | 5-methyl-3-hexanone | 135 | 137.3 | 20.12 | 22.53 | 2.22 | 60.83 | 0.87 | 2.48 | 1.82 | 0.09 | 64.88 | 1274.75 |
| 131 | 2,2-dimethyl-3-pentanone | 125.6 | 127.4 | 21.55 | 26.37 | 1.96 | 89.47 | 0.69 | 2.35 | 1.65 | 0.12 | 56.26 | 12636.15 |
| 132 | 2,4-dimethyl-3-pentanone | 125.4 | 128.8 | 20.97 | 24.29 | 2.05 | 70.73 | 0.7 | 2.4 | 1.71 | 0.11 | 46.75 | 632.45 |
| 133 | 4,4-dimethyl-2-pentanone | 126.4 | 130.6 | 21.34 | 26.77 | 1.86 | 92.54 | 0.57 | 2.32 | 1.57 | 0.14 | 37.89 | 15983.61 |
| 134 | 2-octanone | 172.5 | 170.7 | 22.15 | 23.47 | 2.77 | 54.71 | 1.27 | 2.91 | 2.16 | 0.05 | 79.62 | 5159.84 |
| 135 | 3-octanone | 167.5 | 167.6 | 22.23 | 23.33 | 2.82 | 53.96 | 1.32 | 2.93 | 2.22 | 0.05 | 95.25 | 4651.02 |
| 136 | 4-octanone | 165.5 | 166.1 | 22.23 | 23.33 | 2.82 | 53.96 | 1.32 | 2.93 | 2.22 | 0.05 | 95.25 | 4651.02 |
| 137 | 2-methyl-4-heptanone | 154 | 157.8 | 22.95 | 25.36 | 2.58 | 66.49 | 1.05 | 2.83 | 2.07 | 0.06 | 72.88 | 3605.55 |
| 138 | 3-methyl-4-heptanone | 153 | 157.2 | 23.09 | 25.07 | 2.67 | 64.43 | 1.16 | 2.86 | 2.14 | 0.05 | 90.63 | 2600 |
| 139 | 3-methyl-2-heptanone | 164 | 161.1 | 23.01 | 25.22 | 2.61 | 65.17 | 1.1 | 2.84 | 2.09 | 0.06 | 75 | 2884.44 |
| 140 | 4-methyl-2-heptanone | 160.5 | 161.6 | 22.95 | 25.36 | 2.58 | 66.49 | 1.05 | 2.83 | 2.07 | 0.06 | 72.88 | 3605.55 |
| 141 | 5-methyl-2-heptanone | 166.5 | 161.9 | 22.95 | 25.36 | 2.58 | 66.49 | 1.05 | 2.83 | 2.07 | 0.06 | 72.88 | 3605.55 |
| 142 | 6-methyl-2-heptanone | 167 | 162.2 | 22.87 | 25.51 | 2.52 | 67.23 | 0.99 | 2.82 | 2.01 | 0.07 | 57.25 | 4000 |
| 143 | 2-methyl-3-heptanone | 158 | 158.3 | 23.01 | 25.22 | 2.61 | 65.17 | 1.1 | 2.84 | 2.09 | 0.06 | 75 | 28844.44 |
| 144 | 5-methyl-3-heptanone | 161 | 158.6 | 23.03 | 25.21 | 2.63 | 65.75 | 1.11 | 2.85 | 2.12 | 0.06 | 88.51 | 3250 |
| 145 | 6-methyl-3-heptanone | 163.2 | 159 | 22.95 | 25.36 | 2.58 | 66.49 | 1.05 | 2.83 | 2.07 | 0.06 | 72.88 | 3605 |
| 146 | 3,3-dimethyl-2-hexanone | 151.5 | 150.3 | 24.45 | 29.1 | 2.36 | 94.8 | 0.88 | 2.72 | 1.93 | 0.08 | 66.37 | 51000 |
| 147 | 4,4-dimethyl-2-hexanone | 154.4 | 151.3 | 20.78 | 24.49 | 2.18 | 78.95 | 0.9 | 2.44 | 1.8 | 0.094 | 78.009 | 18031.22 |
| 148 | 5,5-dimethyl-2-hexanone | 146 | 152 | 24.17 | 29.59 | 2.21 | 98.2 | 0.74 | 2.67 | 1.82 | 0.1 | 45.89 | 67812.74 |
| 149 | 2,2-dimethyl-3-hexanone | 146 | 147.8 | 24.38 | 29.2 | 2.32 | 95.13 | 0.87 | 2.7 | 1.9 | 0.08 | 64.26 | 53610.67 |
| 150 | 2,4-dimethyl-3-hexanone | 145 | 149.3 | 20.26 | 22.25 | 2.31 | 58.78 | 0.98 | 2.51 | 1.89 | 0.08 | 82.63 | 919.23 |
| 151 | 2,5-dimethyl-3-hexanone | 147.5 | 149.8 | 23.73 | 27.26 | 2.37 | 77.7 | 0.83 | 2.75 | 1.94 | 0.08 | 52.63 | 2236.06 |
| 152 | 4,4-dimethyl-3-hexanone | 148 | 147.7 | 24.53 | 28.95 | 2.39 | 94.06 | 0.93 | 2.73 | 1.98 | 0.07 | 82 | 48457.45 |
| 153 | 4,5-dimethyl-3-hexanone | 152 | 150.4 | 23.88 | 26.97 | 2.46 | 75.64 | 0.94 | 2.77 | 2.01 | 0.07 | 70.37 | 1612.45 |
| 154 | 5,5-dimethyl-3-hexanone | 146.5 | 148.7 | 24.25 | 29.45 | 2.26 | 97.46 | 0.8 | 2.69 | 1.87 | 0.09 | 61.52 | 64432.01 |
| 155 | 3-ethyl-3-methyl-2-pentanone | 153.8 | 149.6 | 24.6 | 28.86 | 2.41 | 93.73 | 0.94 | 2.74 | 2.01 | 0.07 | 84.12 | 46097.92 |
| 156 | 3-ethyl-4-methyl-2-pentanone | 154 | 150.8 | 23.88 | 26.97 | 2.46 | 75.64 | 0.94 | 2.77 | 2.01 | 0.07 | 70.37 | 1612.45 |
| 157 | 2,2,4-trimethyl-3-pentanone | 135.1 | 139.9 | 25.16 | 31.09 | 2.11 | 106.34 | 0.65 | 2.62 | 1.78 | 0.11 | 44 | 39650.47 |
| 158 | 2-nonanone | 195 | 191.8 | 24.98 | 26.3 | 3.12 | 60.36 | 1.44 | 3.27 | 2.41 | 0.03 | 87.62 | 14594.24 |
| 159 | 3-nonanone | 190 | 188.8 | 25.06 | 26.15 | 3.17 | 59.62 | 1.5 | 3.28 | 2.47 | 0.03 | 103.25 | 13155.07 |
| 160 | 4- nonanone | 187.5 | 187.1 | 25.06 | 26.15 | 3.28 | 59.62 | 1.5 | 3.28 | 2.47 | 0.03 | 103.25 | 13155.07 |
| 161 | 5- nonanone | 188.4 | 186.5 | 25.06 | 26.15 | 3.17 | 59.62 | 1.5 | 3.28 | 2.47 | 0.03 | 103.25 | 13155.07 |
| 162 | 4-methyl-2-octanone | 184 | 182.6 | 25.78 | 28.19 | 2.93 | 72.14 | 1.23 | 3.19 | 2.32 | 0.04 | 80.88 | 10198.03 |
| 163 | 5-methyl-3-octanone | 179 | 179.6 | 25.85 | 28.04 | 2.98 | 71.4 | 1.28 | 3.2 | 2.37 | 0.04 | 96.51 | 9192.38 |
| 164 | 7-methyl-3-octanone | 182.5 | 179.6 | 25.78 | 28.17 | 2.93 | 72.14 | 1.23 | 3.19 | 2.32 | 0.04 | 80.88 | 10198.03 |
| 165 | 3-methyl-4-octanone | 174 | 177.7 | 25.92 | 27.9 | 3.02 | 70.09 | 1.34 | 3.21 | 2.39 | 0.04 | 98.63 | 7353.91 |
| 166 | 2,5-dimethyl-3-heptanone | 166 | 169.8 | 26.64 | 29.94 | 2.77 | 82.61 | 1.06 | 3.12 | 2.24 | 0.05 | 76.26 | 5700.87 |
| 167 | 2,6-dimethyl-3-heptanone | 171.5 | 169.8 | 26.56 | 30.09 | 2.72 | 83.35 | 1.01 | 3.1 | 2.19 | 0.06 | 60.63 | 6324.55 |
| 168 | 3,3-dimethyl-2-heptanone | 173.5 | 171 | 27.28 | 31.93 | 2.69 | 100.46 | 1.05 | 3.07 | 2.18 | 0.05 | 74.37 | 216374.67 |
| 169 | 4,6-dimethyl-2-heptanone | 173 | 175.8 | 26.49 | 30.23 | 2.69 | 84.67 | 0.95 | 3.09 | 2.17 | 0.06 | 58.51 | 7905.69 |
| 170 | 4,6-dimethyl-3-heptanone | 171.5 | 170.6 | 26.64 | 29.94 | 2.77 | 82.61 | 1.06 | 3.12 | 2.24 | 0.05 | 76.26 | 5700.87 |

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 171 | 7-methyl-4-octanone | 178 | 178 | 25.78 | 28.19 | 2.93 | 72.14 | 1.23 | 3.19 | 2.32 | 0.04 | 80.88 | 10198.03 |
| 172 | 2,3-dimethyl-4-heptanone | 167.5 | 169.9 | 26.71 | 29.8 | 2.81 | 81.3 | 1.11 | 3.13 | 2.26 | 0.05 | 78.37 | 4560.7 |
| 173 | 2,6-dimethyl-4-heptanone | 169.4 | 169.9 | 26.49 | 30.23 | 2.69 | 84.67 | 0.95 | 3.09 | 2.17 | 0.06 | 58.51 | 7905.69 |
| 174 | 3,5-dimethyl-4-heptanone | 162 | 168.8 | 26.78 | 29.65 | 2.86 | 80.56 | 1.17 | 3.14 | 2.31 | 0.04 | 94 | 4110.96 |
| 175 | 2,2,4,4-tetramethyl-3-pentanone | 152 | 149.2 | 29.36 | 37.9 | 2.17 | 141.95 | 0.59 | 2.83 | 1.84 | 0.1 | 41.26 | 109858.01 |
| 176 | 2-decanone | 210 | 211.8 | 27.81 | 29.13 | 3.47 | 66.02 | 1.62 | 3.62 | 2.66 | 0.02 | 95.62 | 41278.75 |
| 177 | 3-decanone | 211 | 209.1 | 27.89 | 28.98 | 3.53 | 65.28 | 1.68 | 3.64 | 2.72 | 0.02 | 111.25 | 37208.17 |
| 178 | 4-decanone | 206.5 | 207.3 | 27.89 | 28.98 | 3.53 | 65.28 | 1.68 | 3.64 | 2.72 | 0.02 | 111.25 | 37208.17 |
| 179 | 5-decanone | 204 | 206.4 | 27.89 | 28.98 | 3.53 | 65.28 | 1.68 | 3.64 | 2.72 | 0.02 | 111.25 | 37208.17 |
| 180 | 2-undecanone | 231.5 | 230.8 | 30.64 | 31.96 | 3.83 | 71.68 | 1.8 | 3.97 | 2.91 | 0.01 | 103.62 | 116753.96 |
| 181 | 3-undecanone | 227 | 228.4 | 30.72 | 31.81 | 3.88 | 70.94 | 1.85 | 3.99 | 2.97 | 0.01 | 119.25 | 105240.63 |
| 182 | 5-undecanone | 227 | 225.5 | 30.72 | 31.81 | 3.88 | 70.94 | 1.85 | 3.99 | 2.97 | 0.01 | 119.25 | 105240.6 |
| 183 | 6-undecanone | 226 | 225.2 | 30.72 | 31.81 | 3.88 | 70.94 | 1.85 | 3.99 | 2.97 | 0.01 | 119.25 | 105240.6 |
| 184 | 2,2,6,6-tetramethyl-4-heptanone | 185 | 181 | 34.76 | 44.05 | 2.77 | 157.92 | 0.8 | 3.51 | 2.28 | 0.06 | 51.78 | 2856308.51 |
| 185 | 2-dodecanone | 246.5 | 249 | 33.47 | 34.79 | 4.18 | 77.33 | 1.97 | 4.33 | 3.16 | 0.01 | 111.62 | 330250.07 |
| 186 | 2-methyl-3-undecanone | 233.5 | 235.1 | 34.33 | 36.54 | 4.03 | 87.8 | 1.81 | 4.26 | 3.09 | 0.01 | 107 | 184604.22 |
| 187 | 2-tridecanon | 263 | 266.1 | 36.3 | 37.62 | 4.53 | 82.99 | 2.15 | 4.68 | 3.41 | 0.009 | 119.62 | 934031.7 |
| 188 | 7-tridecanon | 261 | 260.7 | 36.37 | 37.47 | 4.59 | 82.25 | 2.21 | 4.7 | 3.47 | 0.088 | 135.25 | 841924.8 |
| 189 | 2-methyl-3-tridecanone | 267 | 268 | 39.99 | 42.19 | 4.73 | 99.12 | 2.16 | 4.96 | 3.59 | 0.008 | 123.004 | 1476833.8 |
| 190 | 7-ethyl-2-methyl-4-undecanone | 252.5 | 255.7 | 45.06 | 50.8 | 4.64 | 147.43 | 1.89 | 5.12 | 3.63 | 0.008 | 130.64 | 1043598026 |
| 191 | 2-pentadecanone | 294 | 298.7 | 38.82 | 39.33 | 5.006 | 94.3 | 2.5 | 5.06 | 3.69 | 0.006 | 131 | 2988901.46 |
| 192 | 8-pentadecanone | 291 | 293.4 | 42.03 | 43.12 | 5.3 | 93.56 | 2.56 | 5.41 | 3.97 | 0.004 | 151.25 | 6795938.43 |

TABLE 1. Experimental and Calculated BP values and molecular descriptors

The best Linear Correlation for exp is obtained by Sombor dominating energy.

$$exp = +61.001(E_S(G)) + (-28.645) \tag{13}$$

$$n = 192 \; r = 0.951 \; F = 1814.004$$

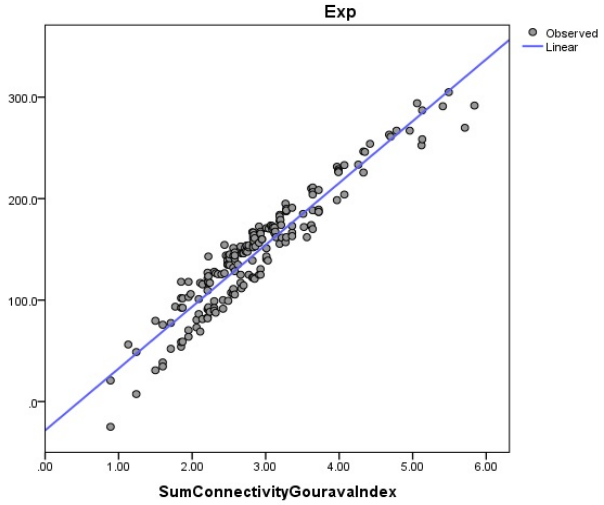


FIGURE 1. linear regression for experimental boiling point

**Conflicts of interest** : The authors declare no conflict of interest.

**Data availability** : Not applicable.

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