

## COMPILATION OF MEASURED YIELD SOOTING INDICES (YSI'S)

This table lists yield sooting indices measured in our group during the past decade [1 – 4]. The YSI of a given test compound is defined by the relation

$$\text{YSI} = A f_{v,\text{max}} + B$$

where  $f_{v,\text{max}}$  is the maximum soot volume fraction measured in a methane/air nonpremixed coflow flame whose fuel is doped with the compound, and A and B are constants chosen so that the YSI's of two endpoint species will have specific values. Given the very wide range of sooting tendencies for the compounds in the database – which range from small oxygenated hydrocarbons to 4-ring PAH – two different sets of endpoints have been used. The table provides a separate listing for each set. For the low sooting tendency species the uncertainties are  $\pm 2$  YSI units, while for the high sooting tendency species they are  $\pm 3$  %. The table includes the CAS Registry number for each test compound; these tags uniquely identify a given substance and were taken from the NIST Chemistry Webbook [1]. Finally, the table lists the paper where each measurement was originally reported.

<u>Species</u>	<u>Formula</u>	<u>CAS #</u>	<u>Ref #</u>	<u>YSI</u>
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### Part I. Low Sooting Tendency Species.

Endpoints = n-hexane (YSI  $\equiv$  0.0) and benzene (YSI  $\equiv$  100.0).

#### *Linear Alkanes*

n-pentane	C <sub>5</sub> H <sub>12</sub>	109-66-0	3	-8.9
n-hexane	C <sub>6</sub> H <sub>14</sub>	110-54-3	3	0.0
2-methylpentane	C <sub>6</sub> H <sub>14</sub>	107-83-5	3	9.8
3-methylpentane	C <sub>6</sub> H <sub>14</sub>	96-14-0	3	12.2
2,2-dimethylbutane	C <sub>6</sub> H <sub>14</sub>	75-83-2	3	20.2
2,3-dimethylbutane	C <sub>6</sub> H <sub>14</sub>	79-29-8	3	21.1
n-heptane	C <sub>7</sub> H <sub>16</sub>	142-82-5	3	8.7
2-methylhexane	C <sub>7</sub> H <sub>16</sub>	591-76-4	3	18.6

3-methylhexane	C <sub>7</sub> H <sub>16</sub>	589-34-4	3	19.6
2,2-dimethylpentane	C <sub>7</sub> H <sub>16</sub>	590-35-2	3	26.5
2,3-dimethylpentane	C <sub>7</sub> H <sub>16</sub>	565-59-3	3	29.6
2,4-dimethylpentane	C <sub>7</sub> H <sub>16</sub>	108-08-7	3	29.9
3,3-dimethylpentane	C <sub>7</sub> H <sub>16</sub>	562-49-2	3	26.9
2,2,3-trimethylbutane	C <sub>7</sub> H <sub>16</sub>	464-06-2	3	38.7
n-octane	C <sub>8</sub> H <sub>18</sub>	111-65-9	3	18.9
2-methylheptane	C <sub>8</sub> H <sub>18</sub>	592-27-8	3	29.5
3-methylheptane	C <sub>8</sub> H <sub>18</sub>	589-81-1	3	28.5
4-methylheptane	C <sub>8</sub> H <sub>18</sub>	589-53-7	3	27.5
2,2-dimethylhexane	C <sub>8</sub> H <sub>18</sub>	590-73-8	3	34.8
2,4-dimethylhexane	C <sub>8</sub> H <sub>18</sub>	589-43-5	3	39.9
2,5-dimethylhexane	C <sub>8</sub> H <sub>18</sub>	592-13-2	3	39.9
3,4-dimethylhexane	C <sub>8</sub> H <sub>18</sub>	583-48-2	3	38.5
2,2,4-trimethylpentane	C <sub>8</sub> H <sub>18</sub>	540-84-1	3	48.6
2,3,4-trimethylpentane	C <sub>8</sub> H <sub>18</sub>	565-75-3	3	47.3
n-nonane	C <sub>9</sub> H <sub>20</sub>	111-84-2	3	30.6
2,3-dimethylheptane	C <sub>9</sub> H <sub>20</sub>	3074-71-3	3	46.3
n-decane	C <sub>10</sub> H <sub>22</sub>	124-18-5	3	41.7
n-undecane	C <sub>11</sub> H <sub>24</sub>	1120-21-4	3	53.3
n-dodecane	C <sub>12</sub> H <sub>26</sub>	112-40-3	3	64.2
2,2,4,6,6-pentamethylheptane	C <sub>12</sub> H <sub>26</sub>	13475-82-6	3	106.9

### *Cyclic Alkanes*

cyclopentane	C <sub>5</sub> H <sub>10</sub>	287-92-3	3	14.0
cyclohexane	C <sub>6</sub> H <sub>12</sub>	110-82-7	3	19.1
methylcyclopentane	C <sub>6</sub> H <sub>12</sub>	96-37-7	3	30.9
cycloheptane	C <sub>7</sub> H <sub>14</sub>	291-64-5	3	30.4
methylcyclohexane	C <sub>7</sub> H <sub>14</sub>	108-87-2	3	36.0
ethylcyclopentane	C <sub>7</sub> H <sub>14</sub>	1640-89-7	3	43.8
cyclooctane	C <sub>8</sub> H <sub>16</sub>	292-64-8	3	42.4
ethylcyclohexane	C <sub>8</sub> H <sub>16</sub>	1678-91-7	3	47.1
1,1-dimethylcyclohexane	C <sub>8</sub> H <sub>16</sub>	590-66-9	3	58.2
cis 1,2-dimethylcyclohexane	C <sub>8</sub> H <sub>16</sub>	2207-01-4	3	54.1
1,3-dimethylcyclohexane	C <sub>8</sub> H <sub>16</sub>	591-21-9	3	57.7

1,4-dimethylcyclohexane	C <sub>8</sub> H <sub>16</sub>	589-90-2	3	57.7
propylcyclohexane	C <sub>9</sub> H <sub>18</sub>	1678-92-8	3	60.3
isopropylcyclohexane	C <sub>9</sub> H <sub>18</sub>	696-29-7	3	68.8
1,2,4-trimethylcyclohexane	C <sub>9</sub> H <sub>18</sub>	2234-75-5	3	81.4
butylcyclohexane	C <sub>10</sub> H <sub>20</sub>	1678-93-9	3	72.0

### *Alkenes*

<i>cis</i> 2-pentene	C <sub>5</sub> H <sub>10</sub>	627-20-3	3	14.7
2-methyl-2-butene	C <sub>5</sub> H <sub>10</sub>	513-35-9	3	20.4
1-hexene	C <sub>6</sub> H <sub>12</sub>	592-41-6	3	18.7
<i>cis</i> 2-hexene	C <sub>6</sub> H <sub>12</sub>	7688-21-3	3	22.3
<i>trans</i> 2-hexene	C <sub>6</sub> H <sub>12</sub>	4050-45-7	3	23.9
<i>trans</i> 3-hexene	C <sub>6</sub> H <sub>12</sub>	13269-52-8	3	26.1
2-methyl-1-pentene	C <sub>6</sub> H <sub>12</sub>	763-29-1	3	19.4
3-methyl-1-pentene	C <sub>6</sub> H <sub>12</sub>	760-20-3	3	22.9
4-methyl-1-pentene	C <sub>6</sub> H <sub>12</sub>	691-37-2	3	30.8
2-methyl-2-pentene	C <sub>6</sub> H <sub>12</sub>	625-27-4	3	36.0
3-methyl-2-pentene	C <sub>6</sub> H <sub>12</sub>	922-61-2	3	36.2
<i>cis</i> 4-methyl-2-pentene	C <sub>6</sub> H <sub>12</sub>	691-38-3	3	36.8
2-ethyl-1-butene	C <sub>6</sub> H <sub>12</sub>	760-21-4	3	23.6
2,3-dimethyl-1-butene	C <sub>6</sub> H <sub>12</sub>	563-78-0	3	35.8
2,3-dimethyl-2-butene	C <sub>6</sub> H <sub>12</sub>	563-79-1	3	49.7
3,3-dimethyl-1-butene	C <sub>6</sub> H <sub>12</sub>	558-37-2	3	35.3
1-heptene	C <sub>7</sub> H <sub>14</sub>	592-76-7	3	27.9
<i>cis</i> 2-heptene	C <sub>7</sub> H <sub>14</sub>	6443-92-1	3	31.7
<i>trans</i> 3-heptene	C <sub>7</sub> H <sub>14</sub>	14686-14-7	3	35.9
2-methyl-1-hexene	C <sub>7</sub> H <sub>14</sub>	6094-02-6	3	29.1
4-methyl-1-hexene	C <sub>7</sub> H <sub>14</sub>	3769-23-1	3	39.4
3-ethyl-2-pentene	C <sub>7</sub> H <sub>14</sub>	816-79-5	3	45.7
4,4-dimethyl-1-pentene	C <sub>7</sub> H <sub>14</sub>	762-62-9	3	48.1
2,3,3-trimethyl-1-butene	C <sub>7</sub> H <sub>14</sub>	594-56-9	3	65.9
1-octene	C <sub>8</sub> H <sub>16</sub>	111-66-0	3	39.8
<i>trans</i> 2-octene	C <sub>8</sub> H <sub>16</sub>	13389-42-9	3	40.8
<i>trans</i> 3-octene	C <sub>8</sub> H <sub>16</sub>	14919-01-8	3	44.1
<i>trans</i> 4-octene	C <sub>8</sub> H <sub>16</sub>	14850-23-8	3	45.6

2-methyl-1-heptene	C <sub>8</sub> H <sub>16</sub>	15870-10-7	3	40.7
2-methyl-2-heptene	C <sub>8</sub> H <sub>16</sub>	627-97-4	3	53.0
2,3,4-trimethyl-2-pentene	C <sub>8</sub> H <sub>16</sub>	565-77-5	3	87.9
2,4,4-trimethyl-1-pentene	C <sub>8</sub> H <sub>16</sub>	107-39-1	3	59.2
2,4,4-trimethyl-2-pentene	C <sub>8</sub> H <sub>16</sub>	107-40-4	3	91.4
1-nonene	C <sub>9</sub> H <sub>18</sub>	124-11-8	3	52.8
1-decene	C <sub>10</sub> H <sub>20</sub>	872-05-9	3	69.0
1-dodecene	C <sub>12</sub> H <sub>24</sub>	112-41-4	3	93.0

#### *Cyclic Alkenes*

cyclopentene	C <sub>5</sub> H <sub>8</sub>	142-29-0	3	61.8
cyclohexene	C <sub>6</sub> H <sub>10</sub>	110-83-8	3	23.7
1-methylcyclopentene	C <sub>6</sub> H <sub>10</sub>	693-89-0	3	102.7
cycloheptene	C <sub>7</sub> H <sub>12</sub>	628-92-2	3	71.6

#### *Alkynes and Alkadienes*

1-pentyne	C <sub>5</sub> H <sub>8</sub>	627-19-0	3	26.2
2-pentyne	C <sub>5</sub> H <sub>8</sub>	627-21-4	3	37.7
2-methyl-1,5-hexadiene	C <sub>7</sub> H <sub>12</sub>	4049-81-4	3	58.0
1-octyne	C <sub>8</sub> H <sub>14</sub>	629-05-0	3	67.8

#### *Saturated Alcohols*

methanol	CH <sub>4</sub> O	67-56-1	3	-36.9
ethanol	C <sub>2</sub> H <sub>6</sub> O	64-17-5	3	-31.1
1-propanol	C <sub>3</sub> H <sub>8</sub> O	71-23-8	3	-22.0
2-propanol	C <sub>3</sub> H <sub>8</sub> O	67-63-0	3	-17.3
1-butanol	C <sub>4</sub> H <sub>10</sub> O	71-36-3	3	-13.0
2-butanol	C <sub>4</sub> H <sub>10</sub> O	78-92-2	3	-8.6
(R)-2-butanol	C <sub>4</sub> H <sub>10</sub> O	14898-79-4	3	-8.1
(S)-2-butanol	C <sub>4</sub> H <sub>10</sub> O	4221-99-2	3	-7.8
2-methyl-1-propanol	C <sub>4</sub> H <sub>10</sub> O	78-83-1	3	-6.5
tert-butanol	C <sub>4</sub> H <sub>10</sub> O	75-65-0	3	-4.5
1-pentanol	C <sub>5</sub> H <sub>12</sub> O	71-41-0	3	-7.7
2-pentanol	C <sub>5</sub> H <sub>12</sub> O	6032-29-7	3	-0.3
3-pentanol	C <sub>5</sub> H <sub>12</sub> O	584-02-1	3	-2.0

2-methyl-1-butanol	C <sub>5</sub> H <sub>12</sub> O	137-32-6	3	3.0
2-methyl-2-butanol	C <sub>5</sub> H <sub>12</sub> O	75-85-4	3	3.9
3-methyl-1-butanol	C <sub>5</sub> H <sub>12</sub> O	123-51-3	3	2.4
3-methyl-2-butanol	C <sub>5</sub> H <sub>12</sub> O	598-75-4	3	4.5
1-hexanol	C <sub>6</sub> H <sub>14</sub> O	111-27-3	3	-0.6
2-hexanol	C <sub>6</sub> H <sub>14</sub> O	626-93-7	3	5.8
3-hexanol	C <sub>6</sub> H <sub>14</sub> O	623-37-0	3	5.5
2-methyl-1-pentanol	C <sub>6</sub> H <sub>14</sub> O	105-30-6	3	8.4
2-methyl-2-pentanol	C <sub>6</sub> H <sub>14</sub> O	590-36-3	3	9.4
3-methyl-1-pentanol	C <sub>6</sub> H <sub>14</sub> O	589-35-5	3	9.2
3-methyl-2-pentanol	C <sub>6</sub> H <sub>14</sub> O	565-60-6	3	11.4
4-methyl-1-pentanol	C <sub>6</sub> H <sub>14</sub> O	626-89-1	3	8.1
4-methyl-2-pentanol	C <sub>6</sub> H <sub>14</sub> O	108-11-2	3	18.1
2-ethyl-1-butanol	C <sub>6</sub> H <sub>14</sub> O	97-95-0	3	17.6
2,3-dimethyl-2-butanol	C <sub>6</sub> H <sub>14</sub> O	594-60-5	3	15.9
3,3-dimethyl-1-butanol	C <sub>6</sub> H <sub>14</sub> O	624-95-3	3	16.3
3,3-dimethyl-2-butanol	C <sub>6</sub> H <sub>14</sub> O	464-07-3	3	15.5
cyclohexanol	C <sub>6</sub> H <sub>12</sub> O	108-93-0	3	18.5
1-heptanol	C <sub>7</sub> H <sub>16</sub> O	111-70-6	3	6.7
2-heptanol	C <sub>7</sub> H <sub>16</sub> O	543-49-7	3	14.0
3-heptanol	C <sub>7</sub> H <sub>16</sub> O	589-82-2	3	12.6
4-heptanol	C <sub>7</sub> H <sub>16</sub> O	589-55-9	3	12.6
2-methyl-2-hexanol	C <sub>7</sub> H <sub>16</sub> O	625-23-0	3	17.8
5-methyl-2-hexanol	C <sub>7</sub> H <sub>16</sub> O	627-59-8	3	22.3
3-ethyl-3-pentanol	C <sub>7</sub> H <sub>16</sub> O	597-49-9	3	15.7
2,2-dimethyl-3-pentanol	C <sub>7</sub> H <sub>16</sub> O	3970-62-5	3	24.2
2,4-dimethyl-3-pentanol	C <sub>7</sub> H <sub>16</sub> O	600-36-2	3	17.9
1-octanol	C <sub>8</sub> H <sub>18</sub> O	111-87-5	3	16.7
2-octanol	C <sub>8</sub> H <sub>18</sub> O	123-96-6	3	24.4
3-octanol	C <sub>8</sub> H <sub>18</sub> O	589-98-0	3	20.6
4-octanol	C <sub>8</sub> H <sub>18</sub> O	589-62-8	3	20.8
2-ethyl-1-hexanol	C <sub>8</sub> H <sub>18</sub> O	104-76-7	3	31.1
2-propyl-1-pentanol	C <sub>8</sub> H <sub>18</sub> O	58175-57-8	3	31.2
2,4,4-trimethyl-1-pentanol	C <sub>8</sub> H <sub>18</sub> O	16325-63-6	3	44.4

*Saturated Ethers*

methyl propyl ether	C <sub>4</sub> H <sub>10</sub> O	557-17-5	3	-19.2
diethyl ether	C <sub>4</sub> H <sub>10</sub> O	60-29-7	3	-21.1
methyl butyl ether	C <sub>5</sub> H <sub>12</sub> O	628-28-4	3	-11.4
methyl sec-butyl ether	C <sub>5</sub> H <sub>12</sub> O	6795-87-5	3	-2.8
methyl tert-butyl ether	C <sub>5</sub> H <sub>12</sub> O	1634-04-4	3	1.7
dipropyl ether	C <sub>6</sub> H <sub>14</sub> O	111-43-3	3	-3.7
diisopropyl ether	C <sub>6</sub> H <sub>14</sub> O	108-20-3	3	12.9
methyl tert-amyl ether	C <sub>6</sub> H <sub>14</sub> O	994-05-8	3	12.0
tert-butyl ethyl ether	C <sub>6</sub> H <sub>14</sub> O	637-92-3	3	11.7
methyl cyclopentyl ether	C <sub>6</sub> H <sub>12</sub> O	5614-37-9	3	49.6
dibutyl ether	C <sub>8</sub> H <sub>18</sub> O	142-96-1	3	12.9
sec-butyl ether	C <sub>8</sub> H <sub>18</sub> O	6863-58-7	3	36.6
isoamyl ether	C <sub>10</sub> H <sub>22</sub> O	544-01-4	3	51.6

*Saturated Alkanones*

2-propanone (acetone)	C <sub>3</sub> H <sub>6</sub> O	67-64-1	3	-26.9
2-butanone	C <sub>4</sub> H <sub>8</sub> O	78-93-3	3	-20.5
2-pentanone	C <sub>5</sub> H <sub>10</sub> O	107-87-9	3	-14.4
3-pentanone	C <sub>5</sub> H <sub>10</sub> O	96-22-0	3	-14.4
3-methyl-2-butanone	C <sub>5</sub> H <sub>10</sub> O	563-80-4	3	-5.9
2-hexanone	C <sub>6</sub> H <sub>12</sub> O	591-78-6	3	-7.4
3-hexanone	C <sub>6</sub> H <sub>12</sub> O	589-38-8	3	-7.6
2-methyl-3-pentanone	C <sub>6</sub> H <sub>12</sub> O	565-69-5	3	0.5
3-methyl-2-pentanone	C <sub>6</sub> H <sub>12</sub> O	565-61-7	3	-2.1
4-methyl-2-pentanone	C <sub>6</sub> H <sub>12</sub> O	108-10-1	3	3.7
3,3-dimethyl-2-butanone	C <sub>6</sub> H <sub>12</sub> O	75-97-8	3	15.8
cyclohexanone	C <sub>6</sub> H <sub>10</sub> O	108-94-1	3	6.1
2-heptanone	C <sub>7</sub> H <sub>14</sub> O	110-43-0	3	0.0
3-heptanone	C <sub>7</sub> H <sub>14</sub> O	106-35-4	3	0.5
4-heptanone	C <sub>7</sub> H <sub>14</sub> O	123-19-3	3	-2.9
2-methyl-3-hexanone	C <sub>7</sub> H <sub>14</sub> O	7379-12-6	3	8.5
2,4-dimethyl-3-pentanone	C <sub>7</sub> H <sub>14</sub> O	565-80-0	3	18.9
4,4-dimethyl-2-pentanone	C <sub>7</sub> H <sub>14</sub> O	590-50-1	3	19.2
2-octanone	C <sub>8</sub> H <sub>16</sub> O	111-13-7	3	11.7

3-octanone	C <sub>8</sub> H <sub>16</sub> O	106-68-3	3	8.8
5-methyl-3-heptanone	C <sub>8</sub> H <sub>16</sub> O	541-85-5	3	20.3
2-nonanone	C <sub>9</sub> H <sub>18</sub> O	821-55-6	3	22.9
3-nonanone	C <sub>9</sub> H <sub>18</sub> O	925-78-0	3	19.6
5-nonanone	C <sub>9</sub> H <sub>18</sub> O	502-56-7	3	17.7
2,6-dimethyl-4-heptanone	C <sub>9</sub> H <sub>18</sub> O	108-83-8	3	39.4
2,2,4,4-tetramethyl-3-pentanone	C <sub>9</sub> H <sub>18</sub> O	815-24-7	3	55.0
2-decanone	C <sub>10</sub> H <sub>20</sub> O	693-54-9	3	33.4
3-decanone	C <sub>10</sub> H <sub>20</sub> O	928-80-3	3	30.7

*Saturated Aldehydes*

propanal (propionaldehyde)	C <sub>3</sub> H <sub>6</sub> O	123-38-6	3	-25.5
butanal	C <sub>4</sub> H <sub>8</sub> O	123-72-8	3	-19.9
isobutanal	C <sub>4</sub> H <sub>8</sub> O	78-84-2	3	-14.3
pentanal	C <sub>5</sub> H <sub>10</sub> O	110-62-3	3	-14.4
2-methylbutanal	C <sub>5</sub> H <sub>10</sub> O	96-17-3	3	-11.9
3-methylbutanal	C <sub>5</sub> H <sub>10</sub> O	590-86-3	3	-3.8
2,2-dimethylpropanal	C <sub>5</sub> H <sub>10</sub> O	630-19-3	3	0.4
hexanal	C <sub>6</sub> H <sub>12</sub> O	66-25-1	3	-5.7
2-methylpentanal	C <sub>6</sub> H <sub>12</sub> O	123-15-9	3	-4.3
2-ethylbutanal	C <sub>6</sub> H <sub>12</sub> O	97-96-1	3	-2.1
3,3-dimethylbutanal	C <sub>6</sub> H <sub>12</sub> O	2987-16-8	3	12.4
heptanal	C <sub>7</sub> H <sub>14</sub> O	111-71-7	3	5.3
octanal	C <sub>8</sub> H <sub>16</sub> O	124-13-0	3	11.1
2-ethylhexanal	C <sub>8</sub> H <sub>16</sub> O	123-05-7	3	9.6
nonanal	C <sub>9</sub> H <sub>18</sub> O	124-19-6	3	20.7
3,5,5-trimethylhexanal	C <sub>9</sub> H <sub>18</sub> O	5435-64-3	3	49.5
decanal	C <sub>10</sub> H <sub>20</sub> O	112-31-2	3	34.8
2-butylhexanal	C <sub>10</sub> H <sub>20</sub> O	18459-51-3	3	27.6

*Cyclic Saturated Ethers*

1,3-dioxolane	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	646-06-0	3	-31.1
tetrahydrofuran	C <sub>4</sub> H <sub>8</sub> O	109-99-9	3	-15.7
1,2-epoxybutane	C <sub>4</sub> H <sub>8</sub> O	106-88-7	3	-17.9
tetrahydropyran	C <sub>5</sub> H <sub>10</sub> O	142-68-7	3	-6.0

2-methoxytetrahydropyran	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	6581-66-4	3	-12.9
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*Saturated Esters and Carboxylic Acids*

ethyl formate	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	109-94-4	3	-32.9
methyl acetate	C <sub>3</sub> H <sub>6</sub> O <sub>2</sub>	79-20-9	3	-29.0
propyl formate	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	110-74-7	3	-15.7
isopropyl formate	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	625-55-8	3	-15.6
ethyl acetate	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	141-78-6	3	-26.4
methyl propionate	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	554-12-1	3	-23.9
butyric acid	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	107-92-6	3	-19.0
isobutyric acid	C <sub>4</sub> H <sub>8</sub> O <sub>2</sub>	79-31-2	3	-17.9
butyl formate	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	592-84-7	3	1.0
isobutyl formate	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	542-55-2	3	0.0
tert-butyl formate	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	762-75-4	3	-0.6
propyl acetate	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	109-60-4	3	-9.3
isopropyl acetate	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	108-21-4	3	-10.4
ethyl propionate	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	105-37-3	3	-15.6
methyl butyrate	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	623-42-7	3	-18.2
methyl isobutyrate	C <sub>5</sub> H <sub>10</sub> O <sub>2</sub>	547-63-7	3	-12.7
pentyl formate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	638-49-3	3	8.3
isopentyl formate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	110-45-2	3	12.1
butyl acetate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	123-86-4	3	8.8
isobutyl acetate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	110-19-0	3	6.9
sec-butyl acetate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	105-46-4	3	7.0
tert-butyl acetate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	540-88-5	3	3.6
propyl propionate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	106-36-5	3	2.4
ethyl butyrate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	105-54-4	3	-7.6
ethyl isobutyrate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	97-62-1	3	-6.6
methyl pentanoate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	624-24-8	3	-12.6
methyl isopentanoate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	556-24-1	3	-3.1
methyl 2-methylbutyrate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	868-57-5	3	-8.5
methyl trimethylacetate	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	598-98-1	3	0.7
2-ethylbutyric acid	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	88-09-5	3	-7.0
2,2-dimethylbutyric acid	C <sub>6</sub> H <sub>12</sub> O <sub>2</sub>	595-37-9	3	-0.6
pentyl acetate	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	628-63-7	3	15.6



isopentyl acetate	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	123-92-2	3	20.6
butyl propionate	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	590-01-2	3	20.1
isobutyl propionate	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	540-42-1	3	16.7
tert-butyl propionate	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	20487-40-5	3	15.7
propyl butyrate	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	105-66-8	3	10.7
isopropyl butyrate	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	638-11-9	3	9.2
ethyl pentanoate	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	539-82-2	3	-3.0
ethyl isopentanoate	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	108-64-5	3	9.7
ethyl 2-methylbutyrate	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	7452-79-1	3	-1.6
methyl hexanoate	C <sub>7</sub> H <sub>14</sub> O <sub>2</sub>	106-70-7	3	-5.7
methyl heptanoate	C <sub>8</sub> H <sub>16</sub> O <sub>2</sub>	106-73-0	3	3.3
methyl octanoate	C <sub>9</sub> H <sub>18</sub> O <sub>2</sub>	111-11-5	3	13.3

*Unsaturated Esters*

methyl-2-propenoate	C <sub>4</sub> H <sub>6</sub> O <sub>2</sub>	96-33-3	4	-17.0
methyl-2-butenolate	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	623-43-8	4	-4.7
methyl-2-methyl-2-propenoate	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	80-62-6	4	-2.2
ethyl-2-propenoate	C <sub>5</sub> H <sub>8</sub> O <sub>2</sub>	140-88-5	4	-13.0
methyl-2-pentenoate	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	15790-88-2	4	5.0
methyl-3-pentenoate	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	818-58-6	4	13.1
methyl-4-pentenoate	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	818-57-5	4	4.5
methyl-2-methyl-2-butenolate	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	6622-76-0	4	11.8
methyl-3-methyl-2-butenolate	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	924-50-5	4	9.4
ethyl-2-butenolate	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	623-70-1	4	-0.1
ethyl-2-methyl-2-propenoate	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	97-63-2	4	-7.7
propyl-2-propenoate	C <sub>6</sub> H <sub>10</sub> O <sub>2</sub>	925-60-0	4	-0.6
methyl-2-hexenoate	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	13894-63-8	4	8.6
methyl-3-hexenoate	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	2396-78-3	4	23.1
methyl-5-hexenoate	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	2396-80-7	4	13.7
methyl-2-methyl-2-pentenoate	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	1567-14-2	4	18.0
ethyl-4-pentenoate	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	1968-40-7	4	16.8
ethyl-2-methyl-2-butenolate	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	5837-78-5	4	5.6
ethyl-3-methyl-2-butenolate	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	638-10-8	4	14.2
propyl-2-methyl-2-propenoate	C <sub>7</sub> H <sub>12</sub> O <sub>2</sub>	2210-28-8	4	10.5

*Other Multi-Oxygen Compounds*

1,2-ethanediol (ethylene glycol)	C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	107-21-1	3	-34.4
1,2-propanediol	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	57-55-6	3	-25.9
dimethyl carbonate	C <sub>3</sub> H <sub>6</sub> O <sub>3</sub>	616-38-6	3	-30.8
dimethoxymethane	C <sub>3</sub> H <sub>8</sub> O <sub>2</sub>	109-87-5	3	-30.3
1,1-dimethoxyethane	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	534-15-6	3	-25.1
1,2-dimethoxyethane	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	110-71-4	3	-28.8
1-methoxy-2-propanol	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	107-98-2	3	-21.7
3-methoxy-1-propanol	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	1589-49-7	3	-19.3
2-ethoxyethanol	C <sub>4</sub> H <sub>10</sub> O <sub>2</sub>	110-80-5	3	-22.8
trimethoxymethane	C <sub>4</sub> H <sub>10</sub> O <sub>3</sub>	149-73-5	3	-27.2
2-hydroxy-methylpropionate	C <sub>4</sub> H <sub>8</sub> O <sub>3</sub>	27871-49-4	3	-32.3
2,2-dimethoxypropane	C <sub>5</sub> H <sub>12</sub> O <sub>2</sub>	77-76-9	3	-21.7
1-methoxy-2-butanol	C <sub>5</sub> H <sub>12</sub> O <sub>2</sub>	53778-73-7	3	-16.4
1,2-dimethoxypropane	C <sub>5</sub> H <sub>12</sub> O <sub>2</sub>	7778-85-0	3	-18.2
2-isopropoxyethanol	C <sub>5</sub> H <sub>12</sub> O <sub>2</sub>	109-59-1	3	-7.5
diethoxymethane	C <sub>5</sub> H <sub>12</sub> O <sub>2</sub>	462-95-3	3	-18.4
2-(2-methoxyethoxy)-ethanol	C <sub>5</sub> H <sub>12</sub> O <sub>3</sub>	111-77-3	3	-23.8
1,1,1-trimethoxyethane	C <sub>5</sub> H <sub>12</sub> O <sub>3</sub>	1445-45-0	3	-27.5
diethyl carbonate	C <sub>5</sub> H <sub>10</sub> O <sub>3</sub>	105-58-8	3	-23.4
1,1-dimethoxy-2-propanone	C <sub>5</sub> H <sub>10</sub> O <sub>3</sub>	6342-56-9	3	-24.2
tetramethoxymethane	C <sub>5</sub> H <sub>12</sub> O <sub>4</sub>	1850-14-2	3	-24.1
2-butoxyethanol	C <sub>6</sub> H <sub>14</sub> O <sub>2</sub>	111-76-2	3	-7.8
diglyme	C <sub>6</sub> H <sub>14</sub> O <sub>3</sub>	111-96-6	3	-22.1
1,1-diethoxyethane	C <sub>6</sub> H <sub>14</sub> O <sub>2</sub>	105-57-7	3	-12.3
3-methoxy-3-methyl-1-butanol	C <sub>6</sub> H <sub>14</sub> O <sub>2</sub>	56539-66-3	3	4.4
1-propoxy-2-propanol	C <sub>6</sub> H <sub>14</sub> O <sub>2</sub>	1569-01-3	3	-7.1
1,2-diethoxyethane	C <sub>6</sub> H <sub>14</sub> O <sub>2</sub>	629-14-1	3	-15.5
1-butoxy-2-propanol	C <sub>7</sub> H <sub>16</sub> O <sub>2</sub>	5131-66-8	3	2.0
1-tert-butoxy-2-propanol	C <sub>7</sub> H <sub>16</sub> O <sub>2</sub>	57018-52-7	3	21.1
1,1-diethoxypropane	C <sub>7</sub> H <sub>16</sub> O <sub>2</sub>	4744-08-5	3	-4.7
dipropyl carbonate	C <sub>7</sub> H <sub>14</sub> O <sub>3</sub>	623-96-1	3	6.4

## Part II. High Sooting Tendency Species.

Endpoints = benzene (YSI  $\equiv$  30.0) and 1,2-dihydronaphthalene (YSI  $\equiv$  100.0).

cyclopentene	C <sub>5</sub> H <sub>8</sub>	142-29-0	1	26.2
benzene	C <sub>6</sub> H <sub>6</sub>	71-43-2	1	30.0
1,3-cyclohexadiene	C <sub>6</sub> H <sub>8</sub>	592-57-4	1	29.7
1,4-cyclohexadiene	C <sub>6</sub> H <sub>8</sub>	628-41-1	1	30.2
cyclohexene	C <sub>6</sub> H <sub>10</sub>	110-83-8	1	22.7
1-methyl-1-cyclopentene	C <sub>6</sub> H <sub>10</sub>	693-89-0	1	29.5
fluorobenzene	C <sub>6</sub> H <sub>5</sub> F	462-06-6	1	31.2
chlorobenzene	C <sub>6</sub> H <sub>5</sub> Cl	108-90-7	1	35.3
bromobenzene	C <sub>6</sub> H <sub>5</sub> Br	108-86-1	1	37.1
toluene	C <sub>7</sub> H <sub>8</sub>	108-88-3	1	43.5
1-methyl-1,4-cyclohexadiene	C <sub>7</sub> H <sub>10</sub>	4313-57-9	1	44.4
methoxybenzene	C <sub>7</sub> H <sub>8</sub> O	100-66-3	1	31.3
2-heptanone	C <sub>7</sub> H <sub>14</sub> O	110-43-0	2	17
cyanobenzene	C <sub>7</sub> H <sub>5</sub> N	100-47-0	1	32.8
phenylacetylene	C <sub>8</sub> H <sub>6</sub>	536-74-3	1	52.2
styrene	C <sub>8</sub> H <sub>8</sub>	100-42-5	1	44.1
ethylbenzene	C <sub>8</sub> H <sub>10</sub>	100-41-4	1	53.6
1,2-dimethylbenzene	C <sub>8</sub> H <sub>10</sub>	95-47-6	1	50.0
1,3-dimethylbenzene	C <sub>8</sub> H <sub>10</sub>	108-38-3	1	53.2
1,4-dimethylbenzene	C <sub>8</sub> H <sub>10</sub>	106-42-3	1	51.2
ethoxybenzene	C <sub>8</sub> H <sub>10</sub> O	103-73-1	1	32.3
(1-propynyl)-benzene	C <sub>9</sub> H <sub>8</sub>	673-32-5	1	92.6
(2-propynyl)-benzene	C <sub>9</sub> H <sub>8</sub>	10147-11-2	1	95.7
1-ethynyl-2-methylbenzene	C <sub>9</sub> H <sub>8</sub>	766-47-2	1	103.6
1-ethynyl-3-methylbenzene	C <sub>9</sub> H <sub>8</sub>	766-82-5	1	84.4
1-ethynyl-4-methylbenzene	C <sub>9</sub> H <sub>8</sub>	766-97-2	1	82.5
indene	C <sub>9</sub> H <sub>8</sub>	95-13-6	1	100.3
(1-propenyl)-benzene	C <sub>9</sub> H <sub>10</sub>	637-50-3	1	78.2
(2-propenyl)-benzene	C <sub>9</sub> H <sub>10</sub>	300-57-2	1	70.3
(1-methylethenyl)-benzene	C <sub>9</sub> H <sub>10</sub>	98-83-9	1	65.6
1-ethenyl-2-methylbenzene	C <sub>9</sub> H <sub>10</sub>	611-15-4	1	88.9

1-ethenyl-3-methylbenzene	C <sub>9</sub> H <sub>10</sub>	100-80-1	1	72.5
1-ethenyl-4-methylbenzene	C <sub>9</sub> H <sub>10</sub>	622-97-9	1	71.8
cyclopropylbenzene	C <sub>9</sub> H <sub>10</sub>	873-49-4	1	76.6
indane	C <sub>9</sub> H <sub>10</sub>	496-11-7	1	94.9
propylbenzene	C <sub>9</sub> H <sub>12</sub>	103-65-1	1	55.9
isopropylbenzene	C <sub>9</sub> H <sub>12</sub>	98-82-8	1	46.7
1-ethyl-2-methylbenzene	C <sub>9</sub> H <sub>12</sub>	611-14-3	1	61.9
1-ethyl-3-methylbenzene	C <sub>9</sub> H <sub>12</sub>	620-14-4	1	64.0
1-ethyl-4-methylbenzene	C <sub>9</sub> H <sub>12</sub>	622-96-8	1	60.0
1,2,3-trimethylbenzene	C <sub>9</sub> H <sub>12</sub>	526-73-8	1	71.1
1,2,4-trimethylbenzene	C <sub>9</sub> H <sub>12</sub>	95-63-6	1	69.8
1,3,5-trimethylbenzene	C <sub>9</sub> H <sub>12</sub>	108-67-8	1	70.3
naphthalene	C <sub>10</sub> H <sub>8</sub>	91-20-3	1	100.0
azulene	C <sub>10</sub> H <sub>8</sub>	275-51-4	2	105
(1-butynyl)-benzene	C <sub>10</sub> H <sub>10</sub>	622-76-4	1	102.8
(3-butynyl)-benzene	C <sub>10</sub> H <sub>10</sub>	16520-62-0	1	68.0
1-ethynyl-4-ethylbenzene	C <sub>10</sub> H <sub>10</sub>	40307-11-7	1	95.5
1-ethynyl-2,5-dimethylbenzene	C <sub>10</sub> H <sub>10</sub>	74331-70-7	1	108.9
2-methylindene	C <sub>10</sub> H <sub>10</sub>	2177-47-1	1	106.5
1,2-dihydronaphthalene	C <sub>10</sub> H <sub>10</sub>	447-53-0	1	100.0
(3-butenyl)-benzene	C <sub>10</sub> H <sub>12</sub>	768-56-9	1	63.6
(2-methyl-1-propenyl)-benzene	C <sub>10</sub> H <sub>12</sub>	768-49-0	1	94.4
1-ethenyl-2,5-dimethylbenzene	C <sub>10</sub> H <sub>12</sub>	2039-89-6	1	100.6
tetralin	C <sub>10</sub> H <sub>12</sub>	119-64-2	1	75.1
dicyclopentadiene	C <sub>10</sub> H <sub>12</sub>	77-73-6	2	41
n-butylbenzene	C <sub>10</sub> H <sub>14</sub>	104-51-8	1	57.7
(1-methylpropyl)-benzene	C <sub>10</sub> H <sub>14</sub>	135-98-8	1	48.9
(2-methylpropyl)-benzene	C <sub>10</sub> H <sub>14</sub>	538-93-2	1	60.1
(1,1-dimethylethyl)-benzene	C <sub>10</sub> H <sub>14</sub>	98-06-6	1	66.5
1,2-diethylbenzene	C <sub>10</sub> H <sub>14</sub>	135-01-3	1	82.8
1,3-diethylbenzene	C <sub>10</sub> H <sub>14</sub>	141-93-5	1	72.2
1,4-diethylbenzene	C <sub>10</sub> H <sub>14</sub>	105-05-5	1	62.6
1-isopropyl-4-methylbenzene	C <sub>10</sub> H <sub>14</sub>	99-87-6	1	74.0
1,2,3,4-tetramethylbenzene	C <sub>10</sub> H <sub>14</sub>	488-23-3	1	86.0
1,2,3,5-tetramethylbenzene	C <sub>10</sub> H <sub>14</sub>	527-53-7	1	84.7

1,2,4,5-tetramethylbenzene	C <sub>10</sub> H <sub>14</sub>	95-93-2	2	86
<i>cis</i> + <i>trans</i> decahydronaphthalene	C <sub>10</sub> H <sub>18</sub>	91-17-8	2	31
1-methylnaphthalene	C <sub>11</sub> H <sub>10</sub>	90-12-0	2	135
2-methylnaphthalene	C <sub>11</sub> H <sub>10</sub>	91-57-6	2	135
n-pentylbenzene	C <sub>11</sub> H <sub>16</sub>	538-68-1	1	59.6
(3-methylbutyl)-benzene	C <sub>11</sub> H <sub>16</sub>	2049-94-7	1	60.2
(2,2-dimethylpropyl)-benzene	C <sub>11</sub> H <sub>16</sub>	1007-26-7	1	63.0
4-tert-butylbenzene	C <sub>11</sub> H <sub>16</sub>	98-51-1	1	89.4
pentamethylbenzene	C <sub>11</sub> H <sub>16</sub>	700-12-9	2	103
acenaphthene	C <sub>12</sub> H <sub>10</sub>	83-32-9	2	165
biphenyl	C <sub>12</sub> H <sub>10</sub>	92-52-4	2	128
1-ethylnaphthalene	C <sub>12</sub> H <sub>12</sub>	1127-76-0	2	151
2-ethylnaphthalene	C <sub>12</sub> H <sub>12</sub>	939-27-5	2	145
1,2-dimethylnaphthalene	C <sub>12</sub> H <sub>12</sub>	573-98-8	2	153
1,3-dimethylnaphthalene	C <sub>12</sub> H <sub>12</sub>	575-41-7	2	153
1,4-dimethylnaphthalene	C <sub>12</sub> H <sub>12</sub>	571-58-4	2	147
1,5-dimethylnaphthalene	C <sub>12</sub> H <sub>12</sub>	571-61-9	2	160
2,3-dimethylnaphthalene	C <sub>12</sub> H <sub>12</sub>	581-40-8	2	154
2,6-dimethylnaphthalene	C <sub>12</sub> H <sub>12</sub>	581-42-0	2	159
1-cyclohexen-1-ylbenzene	C <sub>12</sub> H <sub>14</sub>	771-98-2	2	96
cyclohexylbenzene	C <sub>12</sub> H <sub>16</sub>	827-52-1	2	83
1,5-dimethyltetralin	C <sub>12</sub> H <sub>16</sub>	21564-91-0	2	127
methylcyclopentadiene dimer	C <sub>12</sub> H <sub>16</sub>	26472-00-4	2	47
n-hexylbenzene	C <sub>12</sub> H <sub>18</sub>	1077-16-3	2	58
1,3-diisopropylbenzene	C <sub>12</sub> H <sub>18</sub>	99-62-7	1	78.4
hexamethylbenzene	C <sub>12</sub> H <sub>18</sub>	87-85-4	2	119
fluorene	C <sub>13</sub> H <sub>10</sub>	86-73-7	2	200
bicyclohexyl	C <sub>12</sub> H <sub>22</sub>	92-51-3	2	30
2-methylbiphenyl	C <sub>13</sub> H <sub>12</sub>	643-58-3	2	176
3-methylbiphenyl	C <sub>13</sub> H <sub>12</sub>	643-93-6	2	160
4-methylbiphenyl	C <sub>13</sub> H <sub>12</sub>	644-08-6	2	158
diphenylmethane	C <sub>13</sub> H <sub>22</sub>	101-81-5	2	128
diphenyl ether	C <sub>12</sub> H <sub>10</sub> O	101-84-8	2	57
n-heptylbenzene	C <sub>13</sub> H <sub>20</sub>	1078-71-3	2	60
phenanthrene	C <sub>14</sub> H <sub>10</sub>	85-01-8	2	191

anthracene	C <sub>14</sub> H <sub>10</sub>	120-12-7	2	195
diphenylacetylene	C <sub>14</sub> H <sub>10</sub>	501-65-5	2	133
1,1-diphenylethylene	C <sub>14</sub> H <sub>12</sub>	530-48-3	2	153
<i>cis</i> 1,2-diphenylethylene	C <sub>14</sub> H <sub>12</sub>	645-49-8	2	126
<i>trans</i> 1,2-diphenylethylene	C <sub>14</sub> H <sub>12</sub>	103-30-0	2	126
9,10-dihydroanthracene	C <sub>14</sub> H <sub>12</sub>	613-31-0	2	200
9,10-dihydrophenanthrene	C <sub>14</sub> H <sub>12</sub>	776-35-2	2	193
1-methylfluorene	C <sub>14</sub> H <sub>12</sub>	1730-37-6	2	205
diphenylformaldehyde	C <sub>13</sub> H <sub>10</sub> O	119-61-9	2	72
4-ethylbiphenyl	C <sub>14</sub> H <sub>14</sub>	5707-44-8	2	166
bibenzyl	C <sub>14</sub> H <sub>14</sub>	103-29-7	2	101
2,2'-dimethylbiphenyl	C <sub>14</sub> H <sub>14</sub>	605-39-0	2	199
3,3'-dimethylbiphenyl	C <sub>14</sub> H <sub>14</sub>	612-75-9	2	189
4,4'-dimethylbiphenyl	C <sub>14</sub> H <sub>14</sub>	613-33-2	2	183
cyclopenta[def]phenanthrene	C <sub>15</sub> H <sub>10</sub>	203-64-5	2	262
n-octylbenzene	C <sub>14</sub> H <sub>22</sub>	2189-60-8	2	60
2-phenylindene	C <sub>15</sub> H <sub>12</sub>	4505-48-0	2	189
9-methylantracene	C <sub>15</sub> H <sub>12</sub>	779-02-2	2	237
<i>trans</i> 1,2-diphenylpropene	C <sub>15</sub> H <sub>14</sub>	833-81-8	2	155
dibenzosuberane	C <sub>15</sub> H <sub>14</sub>	833-48-7	2	215
4-propylbiphenyl	C <sub>15</sub> H <sub>16</sub>	10289-45-9	2	168
1,1-diphenylpropane	C <sub>15</sub> H <sub>16</sub>	1530-03-6	2	165
1,3-diphenylpropane	C <sub>15</sub> H <sub>16</sub>	1081-75-0	2	90
2,2-diphenylpropane	C <sub>15</sub> H <sub>16</sub>	778-22-3	2	150
fluoranthene	C <sub>16</sub> H <sub>10</sub>	206-44-0	2	258
pyrene	C <sub>16</sub> H <sub>10</sub>	129-00-0	2	250
1-phenylnaphthalene	C <sub>16</sub> H <sub>12</sub>	605-02-7	2	222
n-nonylbenzene	C <sub>15</sub> H <sub>24</sub>	1081-77-2	2	65
4-butylbiphenyl	C <sub>16</sub> H <sub>18</sub>	37909-95-8	2	173
4,4'-dimethylbibenzyl	C <sub>16</sub> H <sub>18</sub>	538-39-6	2	116
n-decylbenzene	C <sub>16</sub> H <sub>26</sub>	104-72-3	2	65
4-pentylbiphenyl	C <sub>17</sub> H <sub>20</sub>	7116-96-3	2	176
1,2-diphenylbenzene	C <sub>18</sub> H <sub>14</sub>	84-15-1	2	267
1,3-diphenylbenzene	C <sub>18</sub> H <sub>14</sub>	92-06-8	2	257
n-undecylbenzene	C <sub>17</sub> H <sub>28</sub>	6742-54-7	2	67

4-benzyl-biphenyl	$C_{19}H_{16}$	613-42-3	2	239
triphenylmethane	$C_{19}H_{16}$	519-73-3	2	220
n-dodecylbenzene	$C_{18}H_{30}$	123-01-3	2	69
n-tridecylbenzene	$C_{19}H_{32}$	123-02-4	2	72
n-tetradecylbenzene	$C_{20}H_{34}$	1459-10-5	2	74

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