

Supplementary Information

From the test-tube to the test-engine: Assessing the suitability of prospective liquid biofuel compounds

Falk Harnisch*, Ingo Blei, Tatiane Regina dos Santos, Maria Möller, Peter Nilges, Peter Eilts & Uwe Schröder

Table SI -1: Raw data of Figure 2

Substances	Auto ignition temperature/ °C [1-6]	Cetane Number / [-][1, 7]
Hydrocarbons		
Dodecane	200.0	87.0
n-Tridecane	202.0	90.0
n-Pentadecane	202.0	96.0
n-Hexadecane	202.0	100.0
heptadecane	202.0	105.0
n-Heptane	204.0	56.0
n-Nonane	205.0	72.0
n-Decane	208.0	77.0
n-Octane	210.0	64.0
n-Tetradecane	220.0	95.0
n-Hexane	224.0	45.0
1-tetradecene	235.0	79.0
1-nonene	237.0	51.0
1-undecene	237.0	65.0
Undecane	240.0	81.0
1-hexadecene	240.0	88.0
cyclohexane	245.0	13.0
bicyclohexyl	245.0	53.0
n-butylcyclohexane	246.0	47.0
1-octene	250.0	41.0
1-octadecene	250.0	90.0
trans-decalin	255.0	48.0
methylcyclohexane	260.0	20.0
1-heptene	260.0	32.0
1-hexene	265.0	27.0
n-Pentane	285.0	30.0
cyclooctane	290.0	22.0
3-methylpentane	300.0	30.0
2,3-dimethylpentane	337.0	21.0
2,4-dimethylpentane	337.0	29.0
1-n-butyl-naphthalene	360.0	6.0
2,2-dimethylbutane	405.0	24.0
sec-butylbenzene	415.0	6.0
2,4,4-trimethyl-1-pentene	420.0	10.0

Supplementary Information

ethyl benzene	430.0	8.0
1,3-diethylbenzene	450.0	9.0
Isohexadecane	472.0	15.0
1,2-diphenylethane	480.0	1.0
diphenylmethane	485.0	11.0
1,3-dimethylbenzene	525.0	1.0
1-Methylnaphthalene	529.0	0.0
biphenyl	570.0	21.0
alcohols		
1-octadecanol	230.0	81.0
1-hexadecanol	235.0	68.0
1-tetradecanol	240.0	51.0
1-decanol	255.0	50.3
1-octanol	270.0	39.1
2-ethyl-1-hexanol	270.0	23.4
1-heptanol	275.0	28.0
1-dodecanol	275.0	63.6
1-nonanol	277.0	46.2
1-undecanol	277.0	53.2
1-hexanol	284.9	23.3
1-pentanol	300.0	20.0
1-butanol	342.9	17.0
1-propanol	371.0	12.0
sec-butanol	405.0	13.5
iso-Butanol	415.0	15.0
Ethanol	420.0	10.0
Methanol	463.0	3.0
tert-butanol	478.0	15.5
acids and ester		
oleic acid	363.0	46.1
decanoic acid	377.0	47.6
2-Ethoxyethyl acetate	379.0	40.0
ethyl levulinate	425.0	5.0
Dimethyl carbonate	458.0	35.0
ether		
diethyl ether	160.0	160.0
dipentyl ether	171.0	111.0
2-ethoxyethyl ether	174.0	113.0
dibutyl ether	185.0	91.0
Diethylene glycol dimethyl ether	190.0	112.0
Triethylene glycol dimethyl ether	195.0	120.0 [8]
1,2-dimethoxyethane	200.0	90.0
dipropylene glycol monomethyl ether	205.0	42.0
Dipropylene glycol monomethyl ether	205.0	42.0
triethylene glycol monomethyl ether	210.0	75.0
2.5.7.10-tetraoxaundecane	210.0	115.0

Supplementary Information

butylal	220.0	74.0
dimethyl ether	235.0	55.0
dimethoxymethane	235.0	50.0
2-butoxyethanol	238.0	35.0
Dioxolane	274.0	30.0
tripropylene glycol monomethyl ether	277.0	63.0
2-methoxyethanol	286.0	13.0
1-methoxy-2 propanol	287.0	19.0
furanics		
2-Methyltetrahydrofuran	270.0	23.5
2-methylfuran	450.0	17.0
aldehydes and ketones		
octanal	190.0	80.5
3-octanone	330.0	35.2
2-heptanone	393.0	30.0

Table SI-2: Raw data of Figure 3

Substance	H _f / kJ mol ⁻¹ [9, 10]	Cetane Number / [-] [1, 11]
hydrocarbons		
heptadecane	-393.9	105.0
n-Hexadecane	-374.8	100.0
n-Pentadecane	-354.8	96.0
n-Tetradecane	-332.1	95.0
n-Tridecane	-311.5	90.0
Dodecane	-289.4	87.0
Undecane	-270.8	81.0
n-Decane	-249.5	77.0
1-hexadecene	-248.4	88.0
n-Nonane	-228.2	72.0
bicyclohexyl	-215.7	53.0
n-butylcyclohexane	-213.7	46.5
1,3,5-trimethylcyclohexane	-212.1	30.5
n-Octane	-208.5	64.0
2,4-dimethylpentane	-201.6	29.0
2,3-dimethylpentane	-198.7	21.0
n-Heptane	-187.6	56.0
2,2-dimethylbutane	-185.9	24.4
trans-decalin	-182.1	48.0
3-methylpentane	-171.9	30.0
n-Hexane	-166.9	45.0
methylcyclohexane	-154.7	20.0
n-Pentane	-146.9	30.0
cyclohexane	-123.4	13.0
2,4,4-trimethyl-1-pentene	-110.5	10.0
1-octene	-81.3	41.0
1-heptene	-62.3	32.0

Supplementary Information

1-hexene	-43.5	27.0
sec-butylbenzene	-18.4	6.0
1,3-dimethylbenzene	17.3	1.0
ethyl benzene	29.9	8.0
1-Methylnaphthalene	116.9	0.0
diphenylmethane	139.0	11.0
1,2-diphenylethane	142.9	1.0
biphenyl	181.4	21.0
ethers		
Diethylene glycol dimethyl ether	-521.3	112.0
butylal	-501.0	74.0
dipentyl ether	-390.0	111.0
2-methoxyethanol	-376.9	13.0
dimethoxymethane	-348.5	50.0
1.2-dimethoxyethane	-342.8	90.0
dibutyl ether	-332.8	91.0
Dioxolane	-298.0	30.0
diethyl ether	-252.1	160.0
dimethyl ether	-184.1	55.0
alcohols		
1-hexadecanol	-517.0	68.0
1-tetradecanol	-474.8	51.0
1-dodecanol	-436.6	63.6
1-decanol	-396.6	50.3
1-nonanol	-376.5	46.2
2-ethyl-1-hexanol	-365.3	23.4
1-octanol	-355.6	39.1
1-heptanol	-336.5	28.0
1-hexanol	-315.9	23.3
tert-butanol	-312.5	15.5
1-pentanol	-294.6	20.0
sec-butanol	-292.8	13.5
iso-Butanol	-283.8	15.0
1-butanol	-274.9	17.0
1-propanol	-255.1	12.0
ethanol	-234.8	10.0
methanol	-201.0	3.0
acids and ester		
tristearin	-2199.0	85.0
tripalmitin	-2075.0	89.0
triolein	-1843.0	45.0
trilaurin	-1828.0	100.0
diethyl adipate	-891.6	15.0
isobutyl stearate	-827.2	99.3
dibutyl maleate	-821.7	26.5
butyl stearate	-818.0	80.1
propyl stearate	-797.5	69.9
methyl arachidate	-784.1	100.0
decyl caprate	-776.6	81.0

Supplementary Information

butyl palmitate	-776.6	87.0
ethyl stearate	-776.6	86.0
octadecyl acetate	-775.7	90.0
isopropyl palmitate	-774.5	82.6
methyl stearate	-743.1	81.0
ethyl palmitate	-735.5	80.0
hexadecyl acetate	-734.3	86.0
methyl palmitate	-701.7	74.5
butyl oleate	-699.1	61.6
ethyl myristate	-694.5	66.9
propyl laurate	-673.6	71.0
methyl myristate	-660.7	66.2
ethyl oleate	-658.1	53.9
ethyl laurate	-653.1	73.0
acetic acid. dodecyl ester	-651.9	77.0
isopropyl decanoate	-651.0	46.6
oleic acid	-644.3	46.1
propyl decanoate	-632.6	52.9
octyl valerate	-632.6	49.0
methyl oleate	-624.3	55.0
ethyl levulinate	-620.9	5.0
methyl laurate	-619.2	61.4
butyl octanoate	-612.1	39.6
ethyl decanoate	-612.1	51.2
decyl acetate	-610.9	62.0
2-Ethoxyethyl acetate	-610.0	40.0
decanoic acid	-598.3	47.6
methyl decanoate	-578.2	47.2
ethyl octanoate	-570.7	42.2
Dimethyl carbonate	-569.9	35.0
linoleic acid. ethyl ester	-538.1	37.1
methyl octanoate	-536.8	33.6
butyl butanoate	-529.7	17.8
linoleic acid	-524.3	31.4
methyl heptanoate	-516.3	33.5
methyl linoleate	-504.2	42.2
methyl caproate	-495.8	24.0
linolenic acid	-405.0	20.4
linolenic acid. methyl ester	-385.0	22.7
methyl sorbate	-286.0	6.0
ether		
Diethylene glycol dimethyl ether	-521.3	112.0
Butylal	-501.0	74.0
dipentyl ether	-390.0	111.0
2-methoxyethanol	-376.9	13.0
dimethoxymethane	-348.5	50.0
1,2-dimethoxyethane	-342.8	90.0
dibutyl ether	-332.8	91.0
Dioxolane	-298.0	30.0

Supplementary Information

diethyl ether	-252.1	160.0
dimethyl ether	-184.1	55.0
furans		
2-Methyltetrahydrofuran	-225.0	23.5
2-methylfuran	-76.4	17.0
Aldehydes and ketones		
3-octanone	-322.0	35.2
2-heptanone	-300.0	30.0
octanal	-289.0	80.5

Table SI-3: Raw data of Figure 4

substances	$H_{LHV} / \text{kJ g}^{-1}$	H_{LHV} (Dulong) / kJ g^{-1}	H_{LHV} (Boie) / kJ g^{-1}
hydrocarbons			
1-Methylnaphthalene	39.38	40.13	39.02
cyclooctane	39.50	42.23	40.44
diphenylmethane	39.61	40.22	39.08
Benzol	40.19	40.70	39.40
Tetralin	40.58	41.93	40.24
Toluol	40.58	41.58	40.00
1,3-dimethylbenzene	40.86	42.23	40.44
ethyl benzene	40.98	42.23	40.44
1,3-diethylbenzene	41.45	43.13	41.04
sec-butylbenzene	41.50	43.13	41.04
trans-decalin	42.62	45.41	42.58
bicyclohexyl	42.83	45.59	42.71
methylcyclohexane	43.45	46.50	43.32
n-butylcyclohexane	43.51	46.50	43.32
cyclohexane	43.53	46.50	43.32
1-hexadecene	43.92	46.50	43.32
heptadecane	44.02	47.13	43.74
n-Hexadecane	44.04	47.17	43.77
n-Pentadecane	44.08	47.21	43.80
2,4,4-trimethyl-1-pentene	44.08	46.50	43.32
n-Tetradecane	44.11	47.26	43.83
n-Tridecane	44.16	47.32	43.87
2-octene	44.17	46.50	43.32
Dodecane	44.21	47.39	43.92
Undecane	44.26	47.47	43.97
2,2,5-trimethylhexane	44.28	47.68	44.11
1-octene	44.30	46.50	43.32
n-Decane	44.33	47.56	44.03
1-heptene	44.39	46.50	43.32
n-Nonane	44.42	47.68	44.11

Supplementary Information

1-hexene	44.50	46.50	43.32
n-Octane	44.52	47.82	44.21
2,4-dimethylpentane	44.56	48.01	44.34
2,3-dimethylpentane	44.57	48.01	44.34
n-Heptane	44.66	48.01	44.34
2,2-dimethylbutane	44.66	48.25	44.50
3-methylpentane	44.80	48.25	44.50
n-Hexane	44.84	48.25	44.50
n-Pentane	45.08	48.59	44.73
alcohols			
Glycerol	16.06	16.00	16.22
Ethylene glycol	16.98	17.14	17.06
methanol	19.95	20.42	19.47
ethanol	26.86	28.36	26.73
1-propanol	30.77	32.59	30.61
tert-butanol	32.77	35.23	33.01
sec-butanol	32.99	35.23	33.01
iso-Butanol	33.10	35.23	33.01
1-butanol	33.20	35.23	33.01
1-pentanol	34.86	37.02	34.65
1-hexanol	36.05	38.32	35.84
1-heptanol	36.96	39.31	36.74
2-ethyl-1-hexanol	37.64	40.08	37.45
1-octanol	37.69	40.08	37.45
1-nonanol	38.25	40.71	38.02
1-decanol	38.73	41.22	38.49
1-undecanol	39.12	41.65	38.88
1-dodecanol	39.46	42.02	39.22
1-tetradecanol	39.99	42.60	39.75
acids and ester			
methyl formate	14.73	13.64	14.48
methyl acetate	19.73	19.86	19.94
Diethyl malonate	20.11	20.91	21.06
Trimethyl orthoformate	20.89	20.03	19.80
Diethyl carbonate	21.14	21.44	21.33
Ethyl acetoacetate	22.53	22.59	22.57
ethyl acetate	23.43	24.10	23.66
methyl caproate	30.06	31.34	30.02
butyl butanoate	31.20	32.82	31.31
methyl heptanoate	31.36	32.82	31.31
methyl octanoate	32.46	34.03	32.37
decanoic acid	32.97	35.04	33.27
ethyl octanoate	33.28	35.04	33.27
methyl decanoate	34.14	35.91	34.02
ethyl decanoate	34.73	36.65	34.67

Supplementary Information

methyl laurate	35.36	37.29	35.24
ethyl laurate	35.81	37.86	35.74
methyl myristate	36.31	38.36	36.17
ethyl myristate	36.58	38.80	36.56
methyl linoleate	37.22	38.77	36.75
methyl oleate	37.49	39.34	37.13
ether			
Diethylene glycol	20.33	20.03	19.80
Dioxolane	21.24	19.86	19.94
Triethylene glycol	21.66	21.22	20.93
2-methoxyethanol	22.71	22.55	21.90
Diethylene glycol monomethyl ether	22.90	23.12	22.55
dimethoxymethane	23.29	22.55	21.90
Diethylene glycol dimethyl ether	26.10	25.56	24.72
1,2-dimethoxyethane	26.74	26.28	25.23
dimethyl ether	28.47	28.36	26.73
Diethoxymethane	28.55	29.00	27.67
Acetal	30.20	31.08	29.53
butylal	33.83	35.13	33.15
diethyl ether	33.84	35.23	33.01
Isopropyl methyl ether	33.85	35.23	33.01
Methyl propyl ether	34.03	35.23	33.01
TAME	36.40	38.32	35.84
tert-Butyl isopropyl ether	37.05	39.31	36.74
dibutyl ether	38.06	40.08	37.45
furanics			
Furfural	23.41	21.25	22.11
Tetrahydrofurfuryl alcohol	26.87	27.18	26.36
Furan	29.33	27.57	27.60
2,3-Dihydrofuran	31.37	30.27	29.51
THF	32.30	32.82	31.31
aldehydes and ketones			
Ethanal	24.51	24.10	23.66
g-Valerolactone	24.73	25.28	25.00
Cyclohexanone	33.66	34.91	33.46
3-octanone	36.73	38.80	36.56

Table SI-4: Raw data of Figure 5

substances	Lst	$H_{LHV} / \text{kJ g}^{-1}$ [9, 12, 13] ^{*1}
hydrocarbons		
Naphthalin	12.90	39.14
biphenyl	12.96	39.36
1-Methylnaphthalene	13.08	39.50

Supplementary Information

diphenylmethane	13.11	39.76
Benzol	13.23	40.23
1,2-diphenylethane	13.23	40.07
2,6-dimethylnaphthalene	13.23	39.79
Toluol	13.46	40.62
1-n-butyl-naphthalene	13.46	40.47
Tetralin	13.55	40.68
cyclooctane	13.63	39.62
ethyl benzene	13.63	41.04
1,3-dimethylbenzene	13.63	40.91
1,3-diethylbenzene	13.86	41.51
sec-butylbenzene	13.86	41.57
n-hexylbenzene	14.01	41.98
n-octylbenzene	14.12	42.24
n-nonylbenzene	14.16	42.34
n-dodecylbenzene	14.26	42.59
n-tetradecylbenzene	14.31	42.71
trans-decalin	14.45	42.69
1,9-decadiene	14.45	44.04
bicyclohexyl	14.50	42.88
cyclohexane	14.74	43.57
methylcyclohexane	14.74	43.49
1,3,5-trimethylcyclohexane	14.74	43.42
n-butylcyclohexane	14.74	43.60
1-hexene	14.74	44.56
1-heptene	14.74	44.44
1-octene	14.74	44.35
2,4,4-trimethyl-1-pentene	14.74	44.03
2-octene	14.74	44.28
1-nonene	14.74	44.29
1-undecene	14.74	44.19
1-tetradecene	14.74	44.10
1-hexadecene	14.74	44.06
1-octadecene	14.74	44.02
9-methylheptadecane	14.89	44.12
heptadecane	14.90	44.15
n-Hexadecane	14.91	44.18
Isohexadecane	14.91	44.04
n-Pentadecane	14.92	44.20
n-Tetradecane	14.93	44.24
n-Tridecane	14.95	44.27
5-butyl-nonane	14.95	44.28
Dodecane	14.97	44.32
2,2,4,6,6-pentamethylheptane	14.97	44.15
Undecane	14.99	44.36

Supplementary Information

n-Decane	15.01	44.43
2,2-dimethyloctane	15.01	44.33
n-Nonane	15.04	44.50
2,2,5-trimethylhexane	15.04	44.35
n-Octane	15.08	44.59
n-Heptane	15.13	44.71
2,3-dimethylpentane	15.13	44.63
2,4-dimethylpentane	15.13	44.60
n-Hexane	15.19	44.86
2,2-dimethylbutane	15.19	44.71
3-methylpentane	15.19	44.84
n-Pentane	15.28	45.08
alcohols		
Glycerol	5.24	16.33
Ethylene glycol	5.55	17.32
1,3-Formalglycerol	5.96	18.97
methanol	6.45	20.06
ethanol	8.97	26.99
1-propanol	10.32	30.89
1-butanol	11.15	33.34
iso-Butanol	11.15	33.22
sec-butanol	11.15	33.08
tert-butanol	11.15	32.84
1-pentanol	11.72	34.99
1-hexanol	12.14	36.20
1-heptanol	12.45	37.11
1-octanol	12.70	37.82
2-ethyl-1-hexanol	12.70	37.81
3-octanol	12.70	37.69
1-nonanol	12.90	38.40
1-decanol	13.06	38.87
1-undecanol	13.20	39.28
1-dodecanol	13.31	39.61
palmitoleyl alcohol	13.47	40.39
1-tetradecanol	13.50	40.15
oleyl alcohol	13.60	40.75
1-hexadecanol	13.64	40.57
1-octadecanol	13.76	40.90
acids and ester		
Dimethyl carbonate	4.59	14.46
Trimethyl orthoformate	6.49	20.88
methyl acetate	6.51	19.77
Diethyl malonate	6.88	20.75
Diethyl carbonate	7.00	21.19
Diethyl maleate	7.20	22.15

Supplementary Information

Ethyl acetoacetate	7.41	22.44
diethyl succinate	7.52	22.65
2-Ethoxyethyl acetate	7.82	23.96
ethyl acetate	7.82	23.45
Propylene glycol monomethyl ether acetate	7.82	23.92
ethyl levulinate	8.12	24.57
diethyl adipate	8.52	25.58
dibutyl maleate	9.05	27.46
methyl sorbate	9.29	28.88
methyl caproate	10.06	30.10
butyl butanoate	10.51	31.34
methyl heptanoate	10.51	31.43
methyl octanoate	10.89	32.53
decanoic acid	11.20	33.15
ethyl octanoate	11.20	33.36
methyl decanoate	11.47	34.22
butyl octanoate	11.69	34.82
ethyl decanoate	11.69	34.82
trilaurin	11.75	35.02
methyl laurate	11.89	35.47
isopropyl decanoate	11.89	35.32
propyl decanoate	11.89	35.40
octyl valerate	11.89	35.40
acetic acid. dodecyl ester	12.07	35.92
ethyl laurate	12.07	35.92
linolenic acid	12.13	36.81
methyl myristate	12.22	36.42
propyl laurate	12.22	36.37
linolenic acid. methyl ester	12.25	37.32
linoleic acid	12.28	36.99
ethyl myristate	12.36	36.77
tripalmitin	12.38	36.84
methyl linoleate	12.40	37.48
oleic acid	12.44	37.16
triolein	12.45	37.33
methyl palmitate	12.48	37.19
linoleic acid. ethyl ester	12.51	37.72
methyl oleate	12.55	37.64
hexadecyl acetate	12.59	37.47
ethyl palmitate	12.59	37.46
tristearin	12.60	37.50
ethyl oleate	12.65	37.87
methyl stearate	12.70	37.80
isopropyl palmitate	12.70	37.70

Supplementary Information

octadecyl acetate	12.79	38.03
decyl caprate	12.79	38.03
butyl palmitate	12.79	38.03
ethyl stearate	12.79	38.03
butyl oleate	12.82	38.36
methyl arachidate	12.87	38.31
propyl stearate	12.87	38.27
butyl stearate	12.95	38.50
isobutyl stearate	12.95	38.47
ether		
Diethylene glycol	6.49	20.50
methoxy(methoxymethoxy)methane	6.49	21.14
Dioxolane	6.51	21.21
Triethylene glycol	6.88	21.82
dimethoxymethane	7.24	23.34
2-methoxyethanol	7.24	22.90
Diethylene glycol monomethyl ether	7.46	23.67
triethylene glycol monomethyl ether	7.55	24.02
2.5.7.10-tetraoxaundecane	7.55	24.22
Tetraethylene glycol dimethyl ether	8.06	25.70
Triethylene glycol dimethyl ether	8.12	25.87
2(2-Ethoxyethoxy)ethanol	8.22	25.67
Diethylene glycol dimethyl ether	8.22	26.17
1.2-dimethoxyethane	8.41	26.75
1-methoxy-2 propanol	8.41	25.95
dipropylene glycol monomethyl ether	8.83	27.23
Dipropylene glycol monomethyl ether	8.83	27.23
dimethyl ether	8.97	28.45
tripropylene glycol monomethyl ether	9.02	27.78
Diethoxymethane	9.26	28.59
2-ethoxyethyl ether	9.34	29.04
2-butoxyethanol	9.91	30.22
Acetal	9.91	30.20
1-butoxy-2-propanol	10.42	31.52
diethoxybutane	10.84	32.80
dimethoxyhexane	10.84	33.27
diethyl ether	11.15	33.88
Methyl propyl ether	11.15	34.05
Isopropyl methyl ether	11.15	33.82
butylal	11.18	33.90
TAME	12.14	36.42
tert-Butyl isopropyl ether	12.45	37.00
2-ethylhexylal	12.64	37.94
dibutyl ether	12.70	38.14
dipentyl ether	13.06	39.13

Supplementary Information

furanics		
5-HMF	6.56	21.40
Furfural	7.17	23.61
3-Furaldehyde	7.17	23.40
5-(ethoxymethyl)-2-furfural	8.05	25.73
5-Methylfurfural	8.13	26.04
2-Furfuryl methyl ether	8.60	27.59
Tetrahydrofurfuryl alcohol	8.77	27.05
2-(diethoxymethyl)furan	8.91	27.91
Furan	9.11	29.32
furfuryl ethyl ether	9.29	29.28
Methyl tetrahydrofurfuryl ether	9.49	29.53
2,3-Dihydrofuran	9.83	31.14
2-methylfuran	10.07	31.59
THF	10.51	32.38
Dimethylfuran	10.75	33.20
2-Methyltetrahydrofuran	11.20	34.02
aldehydes and ketones		
3-Furaldehyde	7.17	23.40
Ethanal	7.82	24.54
4-Hydroxy-2-butanone	7.82	23.92
Cyclohexanone	11.23	33.77
2-heptanone	12.07	36.05
octanal	12.36	37.14
3-octanone	12.36	36.89

*1: value derived according to [13] from H_f [9] and the heat of vaporization[12].

Table SI-5: Raw data of Figure 6

Substances	L_{st}	H_{LHV} (from H_{LHV} (experimentally)[10]) / $MJ\ m^{-3}$
hydrocarbons		
1-Methylnaphthalene	13.08	3.89
diphenylmethane	13.11	3.91
Benzol	13.23	3.93
Toluol	13.46	3.90
Tetralin	13.55	3.87
cyclooctane	13.63	3.75
1,3-dimethylbenzene	13.63	3.88
ethyl benzene	13.63	3.89
1,3-diethylbenzene	13.86	3.87
sec-butylbenzene	13.86	3.87
trans-decalin	14.45	3.81
bicyclohexyl	14.50	3.82
methylcyclohexane	14.74	3.81

Supplementary Information

n-butylcyclohexane	14.74	3.82
cyclohexane	14.74	3.82
1-hexadecene	14.74	3.85
2,4,4-trimethyl-1-pentene	14.74	3.87
2-octene	14.74	3.88
1-octene	14.74	3.89
1-heptene	14.74	3.89
1-hexene	14.74	3.90
heptadecane	14.90	3.82
n-Hexadecane	14.91	3.82
n-Pentadecane	14.92	3.82
n-Tetradecane	14.93	3.82
n-Tridecane	14.95	3.82
Dodecane	14.97	3.82
Undecane	14.99	3.82
n-Decane	15.01	3.82
2,2,5-trimethylhexane	15.04	3.81
n-Nonane	15.04	3.82
n-Octane	15.08	3.82
2,4-dimethylpentane	15.13	3.81
2,3-dimethylpentane	15.13	3.81
n-Heptane	15.13	3.82
2,2-dimethylbutane	15.19	3.80
3-methylpentane	15.19	3.81
n-Hexane	15.19	3.82
n-Pentane	15.28	3.81
alcohols		
Glycerol	5.24	3.97
Ethylene glycol	5.55	3.95
methanol	6.45	4.00
ethanol	8.97	3.87
1-propanol	10.32	3.85
tert-butanol	11.15	3.80
sec-butanol	11.15	3.82
iso-Butanol	11.15	3.84
1-butanol	11.15	3.85
1-pentanol	11.72	3.84
1-hexanol	12.14	3.84
1-heptanol	12.45	3.84
2-ethyl-1-hexanol	12.70	3.83
1-octanol	12.70	3.84
1-nonanol	12.90	3.83
1-decanol	13.06	3.83
1-undecanol	13.20	3.83
1-dodecanol	13.31	3.83

Supplementary Information

1-tetradecanol	13.50	3.83
acids and ester		
methyl formate	4.59	4.15
Trimethyl orthoformate	6.49	4.16
methyl acetate	6.51	3.92
Diethyl malonate	6.88	3.78
Diethyl carbonate	7.00	3.91
Ethyl acetoacetate	7.41	3.93
ethyl acetate	7.82	3.87
methyl caproate	10.06	3.86
butyl butanoate	10.51	3.84
methyl heptanoate	10.51	3.86
methyl octanoate	10.89	3.85
decanoic acid	11.20	3.81
ethyl octanoate	11.20	3.84
methyl decanoate	11.47	3.85
ethyl decanoate	11.69	3.84
methyl laurate	11.89	3.84
ethyl laurate	12.07	3.84
methyl myristate	12.22	3.84
ethyl myristate	12.36	3.83
methyl linoleate	12.40	3.88
methyl oleate	12.55	3.86
ethers		
Diethylene glycol	6.49	4.05
Dioxolane	6.51	4.22
Triethylene glycol	6.88	4.07
Furfural	7.17	4.22
2-methoxyethanol	7.24	4.05
dimethoxymethane	7.24	4.16
Diethylene glycol monomethyl ether	7.46	3.97
Diethylene glycol dimethyl ether	8.22	4.11
1,2-dimethoxyethane	8.41	4.11
Tetrahydrofurfuryl alcohol	8.77	3.96
dimethyl ether	8.97	4.10
Furan	9.11	4.16
Diethoxymethane	9.26	3.98
2,3-Dihydrofuran	9.83	4.13
Acetal	9.91	3.94
THF	10.51	3.97
diethyl ether	11.15	3.92
Isopropyl methyl ether	11.15	3.92
Methyl propyl ether	11.15	3.94
butylal	11.18	3.91

Supplementary Information

TAME	12.14	3.88
tert-Butyl isopropyl ether	12.45	3.85
dibutyl ether	12.70	3.87
furanics		
Furfural	7.17	4.22
Tetrahydrofurfuryl alcohol	8.77	3.96
Furan	9.11	4.16
2,3-Dihydrofuran	9.83	4.13
THF	10.51	3.97
aldehydes and ketones		
Furfural	7.17	4.22
Ethanal	7.82	4.05
γ -Valerolactone	8.26	3.87
Cyclohexanone	11.23	3.87
3-octanone	12.36	3.84

Table SI-6: Raw data of Figure 7

Substances	C/H ratio	CO ₂ /H _{LHV} g MJ ⁻¹ [9, 12] ^{*1}
hydrocarbons		
n-Pentane	0.42	67.66
n-Hexane	0.43	68.31
2,2-dimethylbutane	0.43	68.53
3-methylpentane	0.43	68.34
n-Heptane	0.44	68.77
2,3-dimethylpentane	0.44	68.89
2,4-dimethylpentane	0.44	68.94
n-Octane	0.44	69.13
n-Nonane	0.45	69.40
2,2,5-trimethylhexane	0.45	69.63
n-Decane	0.45	69.62
2,2-dimethyloctane	0.45	69.78
Undecane	0.46	69.81
Dodecane	0.46	69.96
2,2,4,6,6-pentamethylheptane	0.46	70.23
n-Tridecane	0.46	70.10
5-butylnonane	0.46	70.08
n-Tetradecane	0.47	70.20
n-Pentadecane	0.47	70.30
n-Hexadecane	0.47	70.39
Isohexadecane	0.47	70.60
heptadecane	0.47	70.47

Supplementary Information

9-methylheptadecane	0.47	70.55
cyclohexane	0.50	72.01
methylcyclohexane	0.50	72.14
1,3,5-trimethylcyclohexane	0.50	72.27
n-butylcyclohexane	0.50	71.96
1-hexene	0.50	70.41
1-heptene	0.50	70.61
1-octene	0.50	70.74
2,4,4-trimethyl-1-pentene	0.50	71.26
2-octene	0.50	70.86
1-nonene	0.50	70.84
1-undecene	0.50	70.99
1-tetradecene	0.50	71.15
1-hexadecene	0.50	71.21
1-octadecene	0.50	71.27
bicyclohexyl	0.55	74.06
trans-decalin	0.56	74.56
1,9-decadiene	0.56	72.29
n-tetradecylbenzene	0.59	75.09
n-dodecylbenzene	0.60	75.49
n-nonylbenzene	0.63	76.29
n-octylbenzene	0.64	76.64
n-hexylbenzene	0.67	77.53
1,3-diethylbenzene	0.71	79.00
sec-butylbenzene	0.71	78.89
cyclooctane	0.80	83.71
ethyl benzene	0.80	80.81
1,3-dimethylbenzene	0.80	81.07
Tetralin	0.83	81.83
Toluol	0.88	82.31
1-n-butyl-naphthalene	0.88	82.61
Benzol	1.00	84.03
1,2-diphenylethane	1.00	84.36
2,6-dimethylnaphthalene	1.00	84.95
diphenylmethane	1.08	85.53
1-Methylnaphthalene	1.10	86.20
biphenyl	1.20	87.01
Naphthalin	1.25	87.73
alcohols		
1.3-Formalglycerol	0.13	89.13
ethanol	0.17	70.80
1-propanol	0.25	71.11
1-butanol	0.30	71.24
iso-Butanol	0.30	71.49
sec-butanol	0.30	71.78

Supplementary Information

tert-butanol	0.30	72.32
1-pentanol	0.33	71.34
1-hexanol	0.36	71.39
1-heptanol	0.38	71.44
1-octanol	0.39	71.48
2-ethyl-1-hexanol	0.39	71.51
3-octanol	0.39	71.74
1-nonanol	0.40	71.50
1-decanol	0.41	71.52
1-undecanol	0.42	71.53
1-dodecanol	0.42	71.55
1-tetradecanol	0.43	71.57
1-hexadecanol	0.44	71.59
1-octadecanol	0.45	71.60
palmitoleyl alcohol	0.47	72.51
oleyl alcohol	0.47	72.42
acids and ester		
Trimethyl orthoformate	0.10	79.46
methyl acetate	0.17	90.15
Diethyl carbonate	0.20	87.91
Diethyl malonate	0.25	92.71
2-Ethoxyethyl acetate	0.25	83.38
ethyl acetate	0.25	85.21
Propylene glycol monomethyl ether acetate	0.25	83.53
diethyl succinate	0.29	89.23
Ethyl acetoacetate	0.30	90.42
ethyl levulinate	0.33	86.95
diethyl adipate	0.33	85.07
Diethyl maleate	0.33	92.31
methyl caproate	0.36	78.61
butyl butanoate	0.38	77.90
methyl heptanoate	0.38	77.67
methyl octanoate	0.39	76.96
decanoic acid	0.40	77.08
dibutyl maleate	0.40	84.24
ethyl octanoate	0.40	76.57
methyl decanoate	0.41	75.95
butyl octanoate	0.42	75.72
ethyl decanoate	0.42	75.72
methyl laurate	0.42	75.26
isopropyl decanoate	0.42	75.57
propyl decanoate	0.42	75.39
octyl valerate	0.42	75.39
acetic acid. dodecyl ester	0.43	75.11

Supplementary Information

ethyl laurate	0.43	75.12
methyl myristate	0.43	74.77
propyl laurate	0.43	74.88
ethyl myristate	0.44	74.67
methyl palmitate	0.44	74.39
hexadecyl acetate	0.44	74.32
ethyl palmitate	0.44	74.33
trilaurin	0.45	76.69
methyl stearate	0.45	74.10
isopropyl palmitate	0.45	74.31
octadecyl acetate	0.45	74.05
decyl caprate	0.45	74.06
butyl palmitate	0.45	74.06
ethyl stearate	0.45	74.06
methyl arachidate	0.45	73.87
propyl stearate	0.45	73.95
butyl stearate	0.45	73.84
isobutyl stearate	0.45	73.89
tripalmitin	0.46	75.46
tristearin	0.46	75.04
oleic acid	0.47	75.48
methyl oleate	0.47	74.93
ethyl oleate	0.47	74.84
butyl oleate	0.48	74.55
triolein	0.49	75.89
methyl sorbate	0.50	84.57
linoleic acid	0.50	76.37
methyl linoleate	0.50	75.76
linoleic acid. ethyl ester	0.50	75.64
ether		
Diethylene glycol	0.10	80.90
methoxy(methoxymethoxy)methane	0.10	78.49
dimethoxymethane	0.13	74.33
2-methoxyethanol	0.13	75.75
Triethylene glycol	0.14	80.60
dimethyl ether	0.17	66.15
Dioxolane	0.17	84.02
Diethylene glycol monomethyl ether	0.17	77.39
triethylene glycol monomethyl ether	0.19	78.12
2.5.7.10-tetraoxaundecane	0.19	77.46
1.2-dimethoxyethane	0.20	73.03
1-methoxy-2 propanol	0.20	75.27
2(2-Ethoxyethoxy)ethanol	0.21	76.68
Diethylene glycol dimethyl ether	0.21	75.21
Triethylene glycol dimethyl ether	0.22	76.36

Supplementary Information

Tetraethylene glycol dimethyl ether	0.23	77.05
dipropylene glycol monomethyl ether	0.25	76.35
Dipropylene glycol monomethyl ether	0.25	76.35
Diethoxymethane	0.25	73.89
tripropylene glycol monomethyl ether	0.27	76.79
2-ethoxyethyl ether	0.28	74.72
2-butoxyethanol	0.29	73.95
Acetal	0.29	73.99
diethyl ether	0.30	70.10
Methyl propyl ether	0.30	69.74
Isopropyl methyl ether	0.30	70.23
1-butoxy-2-propanol	0.31	73.93
diethoxybutane	0.33	73.41
dimethoxyhexane	0.33	72.36
butylal	0.35	72.91
TAME	0.36	70.96
tert-Butyl isopropyl ether	0.38	71.64
dibutyl ether	0.39	70.89
dipentyl ether	0.41	71.06
2-ethylhexylal	0.42	72.37
furanics		
Tetrahydrofurfuryl alcohol	0.30	79.67
Methyl tetrahydrofurfuryl ether	0.33	76.99
THF	0.38	75.41
2-Methyltetrahydrofuran	0.40	75.10
2-(diethoxymethyl)furan	0.43	83.37
5-HMF	0.50	97.83
2-Furfuryl methyl ether	0.50	85.37
furfuryl ethyl ether	0.50	83.41
2,3-Dihydrofuran	0.50	80.66
5-(ethoxymethyl)-2-furfural	0.50	88.75
Dimethylfuran	0.63	82.75
2-methylfuran	0.67	84.85
5-Methylfurfural	0.67	92.10
Furfural	0.75	97.01
Furan	0.75	88.21
3-Furaldehyde	0.75	97.87
aldehydes and ketones		
Ethanal	0.25	79.53
4-Hydroxy-2-butanone	0.25	83.52
2-heptanone	0.43	74.83
octanal	0.44	73.93
3-octanone	0.44	74.45
Cyclohexanone	0.50	79.67
3-Furaldehyde	0.75	97.87

Supplementary Information

*1: value derived from H_f [9] and the heat of vaporization[12].

Table SI-7a: Raw data of Figure 8, own measurements Institute of Internal Combustion Engines, TU Braunschweig.

evaporated volume [%]	temperature [°C]					
	Swedish class 1 diesel	US diesel	Fisher-Tropsch-diesel	B10	B100	kerosine
0	184.0	198.7	218.6	164.0	330.0	153.0
2					350.0	
5	197.8	216.3	240.4	190.0	353.0	
10	203.4	221.2	244.6	200.0	354.0	166.0
20	210.4	229.6	257.1	217.0		
30	218.0	239.6	268.8	234.0		
40	226.1	249.7	282.0	250.0		
50	233.5	258.8	294.8	268.0	355.0	177.0
60	242.0	266.2	307.0	285.0		
70	250.2	273.8	317.8	302.0		
80	259.1	282.7	329.0	318.0		
90	270.5	295.6	344.3	330.0		247.0
95	279.9	308.4	356.4	350.1		
100	290.0	320.2	359.6		360.0	283.0

Table SI-7b: Raw data of Figure 8 derived from[10].

pure substances	boiling point [°C]
n-hexadecane	287

References

1. Song, C., C.H. His, and I. Mochida, *Chemistry of diesel fuels*. 2000, New York: Taylor Francis.
2. *The Chemical Database*. 2012, The University of Akron.
3. Yanowitz, J.C., E.; McCormick, R. L. , *Utilization of Renewable Oxygenates as Gasoline Blending Components*. . 2011 Center for Transportation Technologies and Systems Colorado.
4. Andrea Bertola, K.B., *Oxygenated Fuels for Particulate Emissions Reduction in Heavy-Duty DI-Diesel Engines with Common-Rail Fuel Injection*, S.T. Paper, Editor. 2000.
5. *ChemicalLAND21*.
6. Arcoumanis, C., et al., *The potential of di-methyl ether (DME) as an alternative fuel for compression-ignition engines: A review*. Fuel, 2008. **87**(7): p. 1014-1030.
7. Mani Natarajan, E.A.F., David W. Naegeli, Tom Asmus, Wendy Clark, John Garbak, A. Manuel, D. González, Eleanor Liney, William Piel, James P. Wallace *Oxygenates for Advanced Petroleum-Based Diesel Fuels: Part 1. Screening and Selection Methodology for the Oxygenates*, in *Interim Draft Report*. 2001, Southwest Research Institute.
8. Boot, M., et al., *Cyclic Oxygenates: A New Class of Second-Generation Biofuels for Diesel Engines* Energy & Fuels, 2008. **23**(4): p. 1808-1817.

Supplementary Information

9. *National Institute of Standards and Technology (NIST) 2010.*
10. Lide, D.R., *Handbook of Chemistry and Physics*. 81st edition ed. 2000: CRC Press.
11. Mollenhauer, K.T., Helmut *Handbuch Dieselmotoren*. 3. ed. 2007, Berlin Heidelberg New York: Springer.
12. Joback, K.G., *A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques*, in *Massachusetts Institute of Technology, Dept. of Chemical Engineering*,. 1984, Massachusetts Institute of Technology: Cambridge, MA. p. 396.
13. *DIN 51900 resp. ASTM D 240*. Testing of solid and liquid fuels - Determination of gross calorific value by the bomb calorimeter and calculation of net calorific value - Part 1: Principles, apparatus, methods 2000.