

Kovats Indices for C₂-C₁₃ Hydrocarbons and Selected Oxygenates/Halocarbons with 100% Dimethylpolysiloxane Columns

by Randall Bramston-Cook, Lotus Consulting

Identification of hydrocarbons in a chromatogram of ambient air or vehicle exhaust is inherently difficult since well over 300 chemical species can be detected, and the most common detector used for measurement - flame ionization - cannot distinguish any of them other than by retention times. Mass spectrometry helps in picking out specific compounds, but many hydrocarbons have remarkably similar spectra and subtle differences become difficult to sort out which hydrocarbon matches a library of standard spectra. Relative retention indices, commonly called Kovats Indices¹, help to assign labels to eluting peaks in samples of ambient air and vehicle exhaust samples, based on elution relative to nearby n-Alkanes. Since most chromatograms for a wide range of hydrocarbons are generated with temperature programmed conditions, the Kovats Index (*KI*) simplifies to:

$$KI_{unknown} = [t_{r(unknown)} - t_{r(n)}] / [t_{r(N)} - t_{r(n)}] * [100 * (N - n)] + (100 * n)$$

where *n* = number of carbon atoms in the smaller n-alkane, *N* = number of carbon atoms in the larger n-alkane, and *t_r* = retention time of associated compounds. This compilation of Kovats Indices is generated from 11 different gas chromatographs, 15 different chromatograms from related columns with differing dimensions, and dissimilar temperature programs. Remarkably, Kovats Indices remain quite consistent. Peak identifications are made from known standard gas mixtures and from mass spectral interpretations.

	Common Name	IUPAC Name	Average Kovats Index	Standard Deviation	Number of Chromatogram Sources
1		ETHANES	200	=0	11
2	R-134a	1,1,1,2-Tetrafluoroethane	248	-	2
3	Propylene	Propene	286	±7	7
4		PROPANE	300	=0	11
5	R-12	Dichlorodifluoromethane	318	-	1
6		Propadiene	326	-	2
7		Propyne	334	±5	4
8	Isobutane	Methylpropane	359	±2	8
9	Isobutylene	Methylpropene	385	-	1
10		But-1-ene	390	±4	4
11		Buta-1,3-diene	394	±2	8
12		Methanol	~395	±1	3
13	n-Butane	BUTANE	400	=0	11
14		But-1-ene-3-yne	404	±1	4
15		But-2-yne	409	-	1
16		trans-But-2-ene	410	±2	10
17	2,2-Dimethylpropane	Neopentane	414	±2	5
18		But-1-yne	417	-	3
19		Acetic Acid	~418	-	1
20		cis-But-2-ene	422	±3	10
21		Butadiyne	428	-	2
22		But-1,2-diene	441	±2	4
23		3-Methylbut-1-ene	453	±4	6
24		Acetonitrile	~456	-	2
25		Ethanol	~458	-	1
26	Isopentane	Methylbutane	473	±2	10
27	Acetone	Propanone	~479	-	2
28		Penta-1,4-diene	480	-	1
29		But-2-yne	485	±2	5
30	R-11	Trichlorofluoromethane	486	-	1
31		Pent-1-ene	488	±2	10
32	Acrylonitrile	Prop-2-enitrile	~491	-	1
33		2-Methylbut-1-ene	495	±1	5
34	Isopropanol	Propan-2-ol	~496	-	1
35	n-Pentane	PENTANE	500	=0	15
36	Isoprene	Methylbuta-1,3-diene	504	±1	13
37		trans-Pent-2-ene	509	±1	13
38		3,3-Dimethylbut-1-ene	513	±1	4
39		cis-Pent-2-ene	515	±1	13
40		Carbon Disulfide	~517	-	1
41		2-Methylbut-2-ene	519	±2	7
42		trans-Penta-1,3-diene	521	-	1
43		2-Ethyl-3-Methylbut-1-ene	523	-	1
44		3-Methylbuta-1,2-diene	526	-	1
45		Cyclopenta-1,3-diene	528	-	1
46		2,2-Dimethylbutane	533	±2	13
47		cis-Penta-1,3-diene	535	-	1
48		Cyclopentene	548	±5	7
49		4-Methylpent-1-ene	553	±3	7
50		3-Methylpent-1-ene	556	±2	6
51	n-Propanol	Propan-1-ol	~557	-	1
52		Cyclopentane	560	±3	14
53		2,3-Dimethylbutane	563	±2	14
54		2,3-Dimethylbut-1-ene	564	-	1
55	MTBE	2-Methoxy-2-methylpropane	~566	±2	3
56		2-Methylpentane	568	±2	13
57		4-Methyl-trans-pent-2-ene	571	±1	4
58	Methylethylketone	Butan-2-one	~573	±3	3

¹ Kovats, E. (1958). "Gas-chromatographische Charakterisierung organischer Verbindungen. Teil 1: Retentionsindices aliphatischer Halogenide, Alkohole, Aldehyde und Ketone". *Helv. Chim. Acta* 41: 1915–32.; and *Nomenclature of Organic Chemistry* (3 ed.). London: Butterworths. 1971 (3rd edition combined) [1958 (A: Hydrocarbons, and B: Fundamental Heterocyclic Systems), 1965 (C: Characteristic Groups)]. ISBN 0408701447. And en.wikipedia.org/wiki/Kovats_retention_index.

59		4-Methyl-cis-pent-2-ene	574	-	2
60		2-Methylpenta-1,4-diene	580	-	1
61		3-Methylpentane	582	±1	14
62		2-Methylpent-1-ene	588	±1	5
63		Hex-1-ene	589	±3	9
64	Isobutanol	Butan-2-ol	~593	-	1
65		Hexa-1,4-diene	597	-	1
66		2-Ethylbut-1-ene	599	-	1
67	n-Hexane	HEXANE	600	=0	15
68	Di-isopropylether	Di(1-methylethyl)ether	~602	-	1
69		trans- Hex-3-ene	603	±1	6
70		cis-Hex-3-ene	604	±1	4
71		trans-Hex-2-ene	605	±0.2	6
72		2-Methylpent-2-ene	606	±1	3
73		2-Methylpent-1-ene	607	±0.5	6
74		3-Methyl-trans-pent-2-ene	608	±6	4
75		3-Methylcyclopent-1-ene	610	±1	3
76		4,4-Dimethyl-trans-pent-2-ene	611	±1	3
77		3-Methyl-trans-pent-2-ene	612	-	2
78		cis-Hex-2-ene	613	±2	7
79		4,4-Dimethylpent-1-ene	614	-	1
80		3-Methyl-cis-pent-2-ene	619	±2	6
81		trans-Hexa-1,3-diene	621	-	1
82		2,2-Dimethylpentane	623	±1	4
83		Methylcyclopentane	625	±1	14
84		2,3-Dimethylpentane	628	-	1
85		2,4-Dimethylpentane	631	±1	13
86		2,3,3-Trimethylbut-1-ene	632	±2	3
87		2,2,3-Trimethylbutane	634	±1	6
88	Ethyl-t-butylether	2-Ethoxy-2-methylpropane	~637	-	2
89		3,4-Dimethylpent-1-ene	639	±2	3
90		2,4-Dimethylpent-1-ene	642	±3	6
91		1-Methylcyclopent-1-ene	643	±2	4
92		Benzene	649	±2	14
93		3-Ethylpent-1-ene	650	-	1
94		3-Methylhex-1-ene	651	±1	4
95		3,3-Dimethylpentane	653	±2	6
96	n-Butanol	Butan-1-ol	~654	-	1
97		2,4-Dimethylpent-2-ene	655	±2	5
98		2,4-Dimethylpent-1-ene	657	-	1
99		Cyclohexane	658	±2	14
100		2-Methyl-trans-hex-3-ene	660	±0.2	3
101		2-Ethyl-3-methyl-trans-but-1-ene	662	±1	3
102		2-Ethyl-3-methylbutane	663	±1	3
103		4-Methyl-trans-hex-2-ene	666	±2	6
104		2-Methylhexane	668	±1	11
105		2,3-Dimethylpentane	669	±1	14
106		5-Methyl-trans-hex-2-ene	671	-	1
107		1,1-Dimethylcyclopentane	672	±1	3
108	tert-Amylmethylether (TAME)	2-Methoxy-2-methylbutane	673	-	1
109		Cyclohexene	674	±1	7
110		3-Methylhexane	676	±1	14
111		5-Methylhex-2-ene	679	±0.3	3
112		3,4-Dimethyl-cis-pent-2-ene	680	-	1
113		trans-1,3-Dimethylcyclopentane	681	±1	8
114		cis-1,3-Dimethylcyclopentane	684	±1	8
115		3-Ethylpentane	686	±1	5
116		trans-1,2-Dimethylcyclopentane	687	±2	4
117	Isooctane	2,2,4-Trimethylpentane	689	±1	14
118		Hept-1-ene	693	±1	5
119		3-Methyl-trans-hex-3-ene	695	±1	5
120		trans-Hept-3-ene	698	±0.1	6
121	n-Heptane	HEPTANE	700	=0	15
122		cis-Hept-3-ene	702	-	1
123		2,2,4-Trimethylpent-1-ene	703	±2	3
124		2-Methylhex-2-ene	704	±2	4
125		trans-Hept-2-ene	705	±1	6
126		3-Ethyl-cis-pent-2-ene	708	±2	5
127		3-Methyl-cis-hex-2-ene	710	±1	7
128		2,3-Dimethyl-trans-pent-2-ene	712	±1	3
129		cis-Hept-2-ene	714	±1	6
130		3-Methyl-trans-hex-2-ene	716	-	1
131		2,3-Dimethylpent-2-ene	717	-	1
132		3-Ethylcyclopent-1-ene	718	-	1
133		cis-1,2-Dimethylcyclopentane	720	±2	3
134		Methylcyclohexane	721	±3	14
135		1,1,3-Trimethylcyclopentane	722	-	1
136		2,2-Dimethylhexane	723	±1	5
137		2,4,4-Trimethylpent-2-ene	727	±2	5
138		Ethylcyclopentane	731	±2	6
139		2,5-Dimethylhexane	733	±2	8
140		2,2,3-Trimethylpentane	734	-	1
141		2,4-Dimethylhexane	735	±1	6
142		1,2,4-Trimethylcyclopentane	740	±2	6
143		3,3-Dimethylhexane	742	±1	6
144		2,4-Dimethylhex-2-ene	746	±2	3
145		1,2,3-Trimethylcyclopentane	748	±1	6
146		2,3,4-Trimethylpentane	752	±3	14
147	n-Pentanol	Pentan-1-ol	~754	-	1
148	Methylbenzene	Toluene	756	±4	14
149					

150		2,3,3-Trimethylpentane	758	-	1
151		2,3-Dimethylhexane	761	±1	6
152		2-Methyl-3-ethylpentane	762	-	1
153		1,1,2-Trimethylcyclopentane	763	±1	4
154		2-Methylheptane	767	±2	14
155		4-Methylheptane	768	±1	7
156		3-Ethyl-3-methylpentane	770	-	1
157		3,4-Dimethylhexane	772	±1	6
158		3-Methylheptane	775	±2	14
159		3-Ethylhexane	777	±1	5
160		cis-1,3-Dimethylcyclohexane	778	±1	4
161		trans-1,4-Dimethylcyclohexane	779	±1	4
162		1,1-Dimethylcyclohexane	782	-	1
163		trans-1-Ethyl-2-methylcyclopentane	783	±1	4
164		2,2,5-Trimethylhexane	785	±0.4	6
165		trans-1-Ethyl-3-methylcyclopentane	788	±0.5	5
166		cis-1-Ethyl-2-methylcyclopentane	790	±1	5
167		Oct-1-ene	792	±0.5	5
168		cis-1-Ethyl-3-methylcyclopentane	793	±1	4
169		2,2,4-Trimethylhexane	795	±1	6
170		trans-Oct-4-ene	797	±1	6
171		1,2-Dimethylcyclohexane	798	-	1
172	n-Octane	OCTANE	800	=0	15
173		trans-Oct-2-ene	804	-	1
174		trans-1,3-Dimethylcyclohexane	806	-	2
175		cis-Oct-4-ene	808	±1	4
176		2,4,4-Trimethylhexane	811	±1	6
177		cis-Oct-2-ene	815	±1	3
178		2,3,5-Trimethylhexane	818	±1	5
179		2,2-Dimethylheptane	820	±1	4
180		2,4-Dimethylheptane	823	±2	7
181		cis-1,2-Dimethylcyclohexane	827	±2	7
182		2,6-Dimethylheptane	831	±1	6
183		Propylcyclopentane	832	-	1
184		Ethylcyclohexane	833	±1	7
185		3,5-Dimethylheptane	838	±1	7
186		Cyclooctene	839	±1	3
187		1,1,3-Trimethylcyclohexane	841	±1	3
188		1,1,4-Trimethylcyclohexane	844	±1	3
189		2,5-Dimethylheptane	847	±1	4
190		Ethylbenzene	852	±4	14
191	n-Hexanol	Hexan-1-ol	-853	-	1
192		1,3,5-Trimethylcyclohexane	854	±2	7
193		2,3-Dimethylheptane	856	±3	4
194		2-Methyloct-1-ene	858	-	1
195		2-Methyloct-2-ene	859	-	1
196	1,3-Dimethylbenzene	m-Xylene	861	±4	14
197	1,4-Dimethylbenzene	p-Xylene	862	±4	13
198		4-Ethylheptane	863	-	2
199		4-Methyloctane	865	±2	5
200		2-Methyloctane	868	±2	5
201		1,2,3-Trimethylcyclohexane	870	-	1
202		3-Ethylheptane	871	-	1
203		3-Methyloctane	872	±3	7
204		3,3-Diethylpentane	875	-	1
205	Vinylbenzene	Styrene	878	±4	14
206		1,2,4-Trimethylcyclohexane	881	-	2
207		1,1,2-Trimethylcyclohexane	882	-	1
208	1,2-Dimethylbenzene	o-Xylene	883	±4	14
209		2,2,4-Trimethylheptane	884	±1	5
210		cis-1,2,4-Trimethylcyclohexane	887	±1	3
211		1-Ethyl-4-methylcyclohexane	888	±2	6
212		2,2,5-Trimethylheptane	890	±3	7
213		Non-1-ene	894	±2	6
214		(2-Methylpropyl)cyclopentane	896	-	1
215		trans-7-Methyloct-3-ene	897	-	1
216		cis-Non-2-ene	898	-	1
217		trans-Non-3-ene	899	-	1
218	n-Nonane	NONANE	900	=0	15
219		1-Ethyl-1-methylcyclohexane	901	-	1
220		3,3-Dimethyloctane	905	±3	5
221		trans-1-Ethyl-3-methylcyclohexane	911	±1	3
222		cis-1-Ethyl-3-methylcyclohexane	914	-	2
223	Isopropylbenzene	Cumene	916	±3	14
224		4,4-Dimethyloctane	920	±0.5	3
225		2,3-Dimethyloctane	921	±3	7
226		2,2-Dimethyloctane	924	±3	7
227		2,5-Dimethyloctane	929	±2	7
228		Benzaldehyde	932	±2	3
229		2,4-Dimethyloctane	934	±2	7
230		2,6-Dimethyloctane	936	±1	6
231	α-Pinene	(1s,5s)-2,6,6-Trimethylbicyclo[3.1.1]hept-2-ene	945	-	1
232		Propylbenzene	947	±3	14
233	m-Ethyltoluene	1-Ethyl-3-methylbenzene	954	±3	13
234	p-Ethyltoluene	1-Ethyl-4-methylbenzene	956	±3	13
235		1,3,5-Trimethylbenzene	961	±1	7
236		4-Methylnonane	964	±1	7
237		2-Methylnonane	966	±1	7
238		3-Methylnonane	969	±3	3

239	o-Ethyltoluene	1-Ethyl-2-methylbenzene	972	±3	14
240		(Dimethylethyl)benzene	977	±3	4
241	Isobutylbenzene	(1-Methylpropyl)benzene	984	-	1
242		1,2,4-Trimethylbenzene	986	±3	14
243		1-Methyl-2-propylcyclohexane	993	-	1
244		(2-Methylpropyl)benzene	996	±2	7
245		Dec-1-ene	997	±1	3
246	n-Decane	DECANE	1000	=0	15
247		1-Methyl-3-propylbenzene	1003	±1	7
248		1-Methyl-3-(1-methylethyl)benzene	1007	±2	5
249		1,2,3-Trimethylbenzene	1015	±4	13
250		1-Methyl-4-(1-methylethyl)benzene	1016	±2	7
251	β-Pinene	6,6-Dimethyl-2-methylenebicyclo[3.1.1]heptane	1017	-	1
252	Benzocyclopentane	Indane	1026	±2	7
253		1-Methyl-2-(1-methylethyl)benzene	1032	±3	6
254	Benzocyclopentadiene	1H-Indene	1033	-	1
255		3-Ethylnonane	1034	-	1
256	m-Diethylbenzene	1,3-Diethylbenzene	1039	±3	7
257		1-Methyl-3-propylbenzene	1042	±3	7
258	p-Diethylbenzene	1,4-Diethylbenzene	1045	±3	12
259		1-Methyl-4-propylbenzene	1047	±3	5
260		1-Ethyl-3,5-dimethylbenzene	1049	±2	6
261		Butylbenzene	1051	±0.5	3
262	o-Diethylbenzene	1,2-Diethylbenzene	1053	±3	12
263	Decalin	1,2,3,4,4a,5,6,7,8,8a-Decahydronaphthalene	1055	-	1
264		1-Methyl-2-propylbenzene	1060	±2	6
265		2-Methyldecane	1067	±1	3
266		1-Ethyl-2,5-dimethylbenzene	1071	±1	6
267		1-Ethyl-2,4-dimethylbenzene	1073	±2	6
268		1-Ethyl-3,4-dimethylbenzene	1079	±2	7
269		1-Ethyl-2,6-dimethylbenzene	1086	±4	7
270		Undec-1-ene	1093	-	1
271		1-Methyl-4-(dimethylethyl)benzene	1094	-	1
272		1-Ethyl-2,3-dimethylbenzene	1095	-	1
273		1-Ethyl-2-(1-methylethyl)benzene	1098	-	1
274	n-Undecane	UNDECANE	1100	=0	14
275		1-Ethyl-4-(methylethyl)benzene	1102	±2	4
276		1-Ethyl-2,3-dimethylbenzene	1106	-	1
277		1,2,4,5-Tetramethylbenzene	1111	±2	7
278		1-Butyl-2-methylbenzene	1113	-	1
279		1,2,3,5-Tetramethylbenzene	1114	±2	6
280		1-Methyl-4-(dimethylethyl)benzene	1117	±0.1	3
281		1-Methyl-2-(dimethylethyl)benzene	1120	±2	4
282	(2,2-Dimethylpropyl)benzene	Neopentylbenzene	1131	±2	3
283		5-Methylindane	1133	±3	6
284		4-Methylindane	1138	±4	5
285		1-Ethyl-2-propylbenzene	1141	-	1
286		1-Methyl-2-(2-methylpropyl)benzene	1143	±5	4
287		2-Methylindane	1145	±5	6
288		1,2,3,4-Tetramethylbenzene	1148	±5	5
289		Pentylbenzene	1150	±1	5
290		1-Butyl-3-methylbenzene	1154	-	1
291		1,3-Diethyl-4-methylbenzene	1157	±1	3
292		2-Methylundecane	1162	±2	3
293		1-Butyl-2-methylbenzene	1165	±4	5
294	Benzocyclohexane	1,2,3,4-Tetrahydronaphthalene	1169	-	1
295	Naphthalene	Bicyclo[4.4.0]deca-1,3,5,7,9-pentene	1173	±4	6
296		1,3-Dimethyl-5-(dimethylethyl)benzene	1176	±4	4
297		1-Butyl-4-ethylbenzene	1181	-	1
298		1,3-Dipropylbenzene	1190	±3	6
299		Dodec-1-ene	1193	-	1
300		DODECANE	1200	=0	8
301		1,3,5-Triethylbenzene	1214	-	1
302		1-Methyl-4-pentylbenzene	1236	-	1
303		1,2,4-Triethylbenzene	1249	-	1
304		Hexylbenzene	1262	-	1
305		1,2,3,4,5-Pentamethylbenzene	1287	-	1
306		2-Methylnaphthalene	1292	-	1
307		Tridec-1-ene	1295	-	1
308		1-Methylnaphthalene	1299	-	1
309		TRIDECANE	1300	=0	7

- Listed compound names follow IUPAC protocol (see: en.wikipedia.org/wiki/IUPAC_nomenclature). For example: Isobutane or 2-Methylpropane is simply **Methylpropane**, as the methyl group can only be substituted in the second position with propane.
- Retention times for Oxygenates, including alcohols and ethers, can vary significantly with differing temperature programs; Kovats indices listed here are approximations only, and should be used only as rough guidelines for their elution.
- Suggested column conditions - Column: Varian CP-Sil 5 CB, 60 meters, 0.25 mm ID, 1 micron film thickness; temperature program: -45 °C, hold for 1.45 minutes, 3.6 °C/minute to 210 °C, hold for 2.72 minutes; flow: 2.0 ml/minute.

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Lotus Consulting

310/569-0128 Fax 714/898-7461
email ebramstoncook@msn.com



5781 Campo Walk
Long Beach, California 90803