Supporting Information for:

Indications of Transformation Products from Hydraulic Fracturing Additives in Shale Gas Wastewater

Kathrin Hoelzer[1†], Andrew J. Sumner[2†], Osman Karatum[3], Robert K. Nelson[4], Brian D. Drollette[2], Megan P. O'Connor[3], Emma L. D'Ambro[5], Gordon J. Getzinger[6], P. Lee Ferguson[3,6], Christopher M. Reddy[4], Martin Elsner[1], Desiree L. Plata[2*]

[1]Helmholtz Zentrum München, Institute of Groundwater Ecology, Ingolstaedter Landstr. 1, 85764 Neuherberg, Germany.

[2]Yale University, School of Engineering and Applied Science, 9 Hillhouse Avenue, New Haven, CT 06511 USA

[3]Duke University, Department of Civil & Environmental Engineering, Hudson Hall, Box 90287, Durham, NC 27705, USA.

[4]Woods Hole Oceanographic Institution, Fye Laboratory, Mail Stop #4, Woods Hole, MA 02543 USA

[5]Department of Chemistry, University of Washington, Seattle, WA 98195 USA.

[6]Duke University, Nicholas School of the Environment, Durham, NC 27705, USA.

[†]Co-first author

*Corresponding author e-mail: desiree.plata@yale.edu ; fax (203) 432-4387; phone (203) 436-9066

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Analytical details

All glassware was combusted in a muffle furnace for 8 hr at 450°C. Glass syringes with metal needles and plungers were used for sample transfer and preparation of standards and were rinsed with high purity solvents (hexane, dichloromethane (DCM), acetone, methanol) and HPLC-grade water prior to use.

Purge-and-trap (P&T): Following a modified EPA 624 method, 5-mL aliquots of the water sample were manually injected with a glass micro-mate syringe (Cadence Science Inc., RI, USA) into a 5-mL Tekmar glass sparger on a Teledyne Tekmar Stratum Purge& Trap (Mason, OH, USA). At ambient temperature, the samples were purged for 4 min with purified Helium (Agilent Big Universal Trap Superior Helium Purifier (RMSH2)) at a purge flow of 40 mL min-1. Dry Purge time was 1.0 min at 40°C at a dry purge flow of 100 mL min-1. Measurements were carried out in triplicate.

GC: Wide-bore, thick phase columns were employed to achieve maximum separation of volatile compounds (DB-624 (60m x 320 um x 1.8 µm; flow: 6mL min-1; T 40°C, 2 min hold, ramp 4°C min-1to 150°C, then ramp 8°C min-1 to 200°C) or Restek-502.2 (105 m x 320um x 3µm; flow: 20 mL min-1; T 40°C, 6 min hold, ramp 6°C min-1to 200°C)).

FID: The FID was set to a temperature of 300°C and operated with a H2 flow of 30 mL min-1, an air flow of 400mL min-1, and a makeup gas flow (He) of 25 mL min-1. VOCs were identified and quantified by comparison with standard reference compounds (502.2 CAL 2000 Mega-Mix (no. 30431), 624 Calibration Mix #1 (no. 30020), 624 Calibration Mix #2 (no. 30021), 624 Calibration Mix #3 (no. 30022), all by Restek, Bellefonte, PA, USA).

LLE: The LLE method entailed adding benzophenone (500 pg) recovery standard to a 113-133 mL water sample and an equivalent volume of 90:10 (v/v) dichloromethane (DCM):methanol. The extraction procedure was repeated twice, using half of the volume of the initial sample volume. After drying with Na_2SO_4, the extracts were rotary evaporated to approximately 1 mL, and filtered through precombusted silica gel columns (constructed in 5-cm Pasteur pipettes preconditioned and washed with 10 and 20 mL DCM, respectively). Note that dilute polar compounds may not have eluted from the silica gel. The eluent was concentrated to approximately 1 mL prior to analysis via GC×GC-TOF-MS and GC×GC-FID.

GC×GC: These analyses were performed at the Woods Hole Oceanographic Institution on a LECO Pegasus 4D (St. Joseph, MI, USA). The primary column was a Restek RXI-1MS (60m length x 250µm d. x 0.25µm film thickness; 50°C, 15 min hold, 1.75°C min^{-1} ramp to 330°C) and the secondary column was an SGE BPX50 (1.5m (0.21 m in the transfer line) x 100µm x 0.10µm; +5°C offset from the primary column and a 10 s modulation) under a flow rate of 1mL min^{-1} without a split. The MS sampled an m/z range of 40-550 amu at a rate of 50 spectra/second.

Confidence assignment: Retention Index Verification

The NIST Mass Spectral Library with Search Program (Data Version: NIST 14, Software Version: 2.2) was used to collect experimental and estimated Retention Index data for all available compounds detected in this study. Based on our own n-alkane standards (n-C7 to n-C36), we calculated experimental Retention Indices for each of the compound detections that passed the 85% similarity and reverse criteria. Retention Indices from NIST and calculated were both based on the "Kovats retention index" for temperature programmed chromatography:

$$I = 100\times\left[n + \frac{t_{r(analyte)} - t_{r(n)}}{t_{r(N)} - t_{r(n)}}\right] \qquad Eq.\ S1$$

where n is the number of carbon atoms in the n-alkane eluting before the analyte, N is the number of carbon atoms in the alkane eluting after the analyte, and t_r is the 1st dimension retention time in seconds.

Retention agreements within ± 100 were classified as positive confidence. The wide tolerance threshold was chosen to allow for enough deviation from NIST database (e.g., to account for experimental and configurational variances) while still narrow enough to reject misidentifications and outliers.

Confidence assignment: Boiling point ladder construction and approach.

First, the CAS registry number (Chemical Abstracts Services) of the best NIST library match (i.e., with the highest forward and reverse similarity) was used to populate an inventory of theoretical and experimental boiling points. Then, a simple linear regression model of boiling point versus 1D retention time was developed using an n-alkane standard ladder ($R^2 = 0.9998$). Boiling points of the tentative mass spectral assignments were run through the algorithm, calculating a predicted 1D retention time. This predicted value was compared to the actual 1D retention time of the detected peak. Agreements within a tolerance of 323 seconds of the predicted retention time (derived from either the theoretical or experimental boiling points) were classified as positive confidence assignments (CA). The tolerance threshold was based off of the mean difference in retention times between standard n-alkanes. This value was chosen to allow for enough deviation from the n-alkane ladder (e.g., as should be the case for distinct compound classes) while still narrow enough to reject misidentifications and outliers.

When possible, we constructed similar standard ladders composed of additional chemical compound classes: specifically, for alcohols, aldehydes, carboxylic acids, and sulfurous acid esters. Tentative identifications were divided manually into chemical classes and run through their respective standard ladder linear models. Note that compounds that did not fall under one of the listed classes deferred to the original n-alkane ladder. As expected,

deviations in chemical behavior led to differing relationships between boiling point and 1D retention time. However, most of the observed deviations were not large, with the notable exception being the carboxylic acid ladder. This was not surprising, since the hydrogen bonding within carboxylic acids leads to enhanced intermolecular interactions relative to n-alkanes, affecting compound's ability to transit the column. Thus, the carboxylic acid ladder was retained in the final linear model and applied to all carboxylic acids, aldehydes, and sulfurous acid esters to better capture these compounds' behaviors; the n-alkane ladder was used for all remaining compounds.

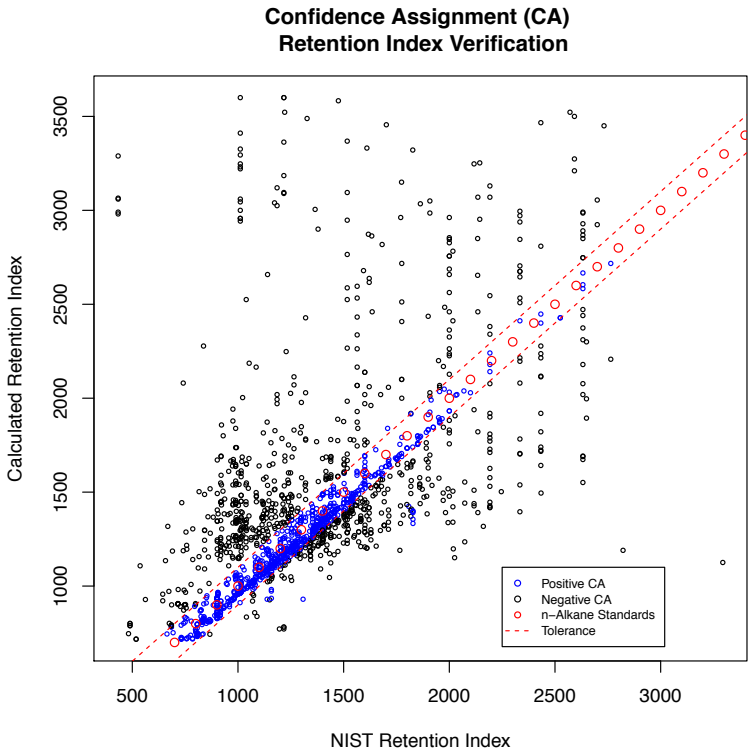

Figure S1a. Retention Index Verification Confidence Assignment Plot.
Confidence Assignments (CA) were made by comparing a calculated Kovats Retention Index value to the NIST Library Database. Positive assignments showed agreement between the top NIST library hit from TOF-MS spectral matching and the calculated retention index (± 100 tolerance shown by "Tolerance" dashed lines). Note that some confidence assignments were made via confirmation with authentic standards

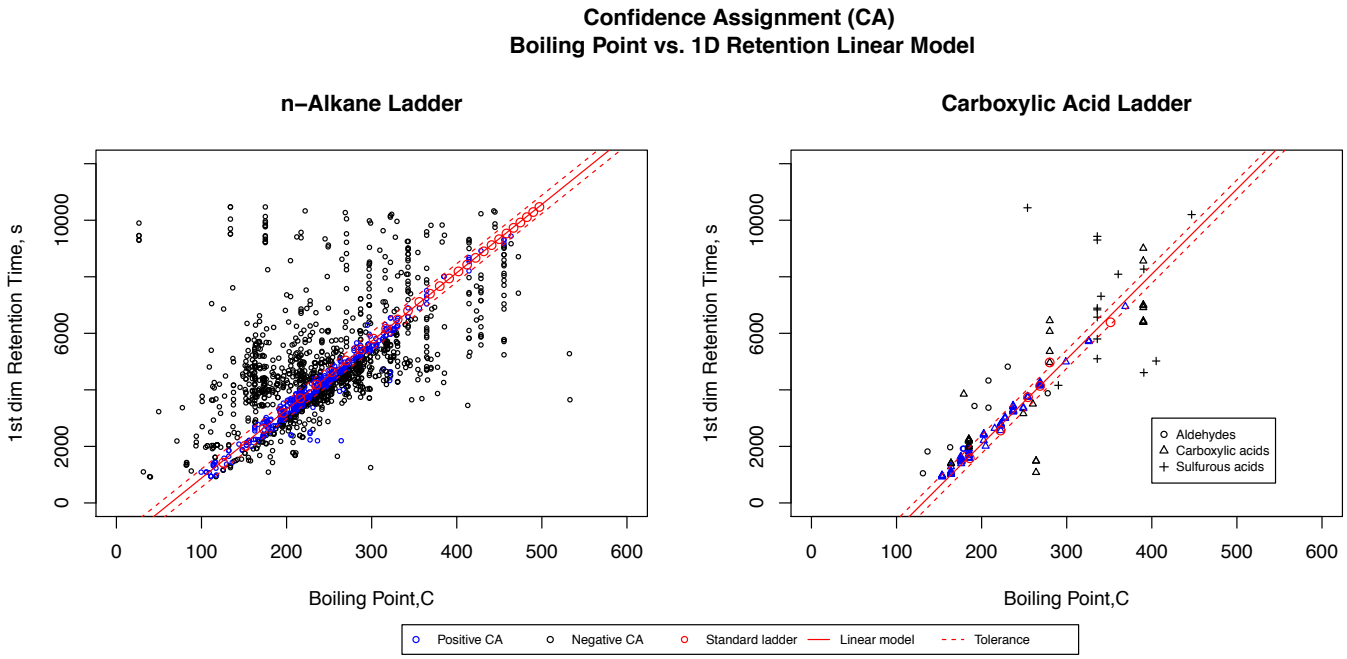

Figure S1b. Boiling Point vs. 1D Retention Model Confidence Assignment Plots. Confidence assignments (CA) were made by applying a predictive linear model relating boiling point and retention time (solid line), constructed using a standard ladder of known compounds. Positive assignments showed agreement between the top NIST library hit from TOF-MS spectral matching and the predicted retention time (± 323 s, tolerance shown by "Tolerance" dashed lines). Unique standard ladders were chosen to help reflect the types of chemical interactions available to each compound class. Note that some confidence assignments were made via confirmation with authentic standards

Control experiments.

Experiment I. Experiments to exclude compound formation or leaching during sample storage. In addition to using standard blank procedures, we conducted three sets of control experiments to ensure that sample collection and storage methods were not a source of analytes. In particular, we probed the potential generation of halogenated or volatile organic compounds in (a) the presence and absence of highly saline water and a model organic compound (acetone) in VOA vials, (b) the presence and absence of actual flowback water samples and a model organic compound (acetone) in an all-glass volumetric flask system, and (c) in the presence of low and high salinity water in representative HDPE bottles similar to the ones initially used by the Arkansas Oil and Gas commission. Synthetic brines (for (a) and (c)) were generated using a recipe of 5.96 g NaHCO3, 7.54 g CaCl2, 34.07 g NaCl, 2.21 g MgCl2, and 1.30 g MgBr2 in 4.0 L of HPLC-grade water. ("Low salt" samples were generated from a 50% dilution of this stock solution). Samples associated with (a) and (b) were acidified with 1 mL of 50% v/v HCl. All experiments were conducted from 0-30 days and analyzed via GC-MS for non-target screening ((a) and (b)) or GC-FID for a target subset of analytes (c). In all analyses, no unexpected halogenated compounds formed.

Experiment II. Experiments to exclude leaching of phthalates into the sample by HDPE bottles. Following the procedure outlined in Experiment I (above), low and high salinity solutions were added to representative, new (i.e., maximum phthalate) HDPE bottles and equilibrated over a period greater than 120 days prior to LLE-GCxGC-TOF-MS analysis. We note that diffusion into and out of polyethylene by phthalates is very slow (> 6 months); see calculations in Drollette et al.[1] and the sample water was in the HDPE containers for much less time (estimated less than 7 days). No phthalates were detected above 7 part per billion detection limit, as confirmed with authentic standards for diisopropyl-, dibutyl-, diethylhexyl- phthalates and phthalic acid.

Here, we caution that no thermal treatment was delivered to the sample containers to simulate a potential influence of heat on the leaching of unique phthalates in each samples. However, we note that (a) the temperature of flowback and produced waters once they reach the surface is often 40°C or less and (b) in order for unique phthalates to be observed in each sample (as shown in our results; see Figure 1 in the main text), then matrix effects unique to each individual sample would have to encourage enhanced transport of individual phthalates, but not others, into the aqueous phase of the sample container. We consider this later scenario highly unlikely for several reasons (i.e., salts generally encourage partitioning to HDPE not vice versa[2] and the physicochemical properties of each of the phthalates would not encourage such compound-specific behavior in each case), and thus, we expect the detected phthalates are authentic to the samples and not an artifact of the collection approach.

Experiment III. Experiments to investigate mass loss over time in VOA vials. EPA standard compounds (see SI above; high molecular weight compounds simulated using 502.2 CAL 2000 Mega-Mix (no. 30431); low molecular weight compounds using 624 Calibration Mix #1 (no. 30020); Restek, Bellefonte, PA, USA) were spiked to HPLC grade water in the VOA vials and measured quantitatively on the GC-FID over 28 days. Losses were less than 5% for low molecular weight compounds and negligible for high molecular weight compounds.

Table S1: Full list of mass spectral library matching-derived tentative identifications and putative compound origins. In columns labeled Sample A-F, an entry corresponds to detection in the respective sample. Y (yes) or N (no) indicates whether a positive confidence assignment could be made based on estimated (est) or experimental (exp) Retention Index (RI) data from the NIST Database. Y' or N' indicates whether a positive confidence assignment could be made based on T (theoretical) or E (experimental) Boiling Points (BP). An entry of "NA" represents a detection without available retention index or boiling point information. Note that some redundancies exist due to the library search software assigning different synonymous names to identical compounds (e.g. "eicosane" and 'n-C20").

***Note**: Table S1 appears at the end of this document, due to its large size.*

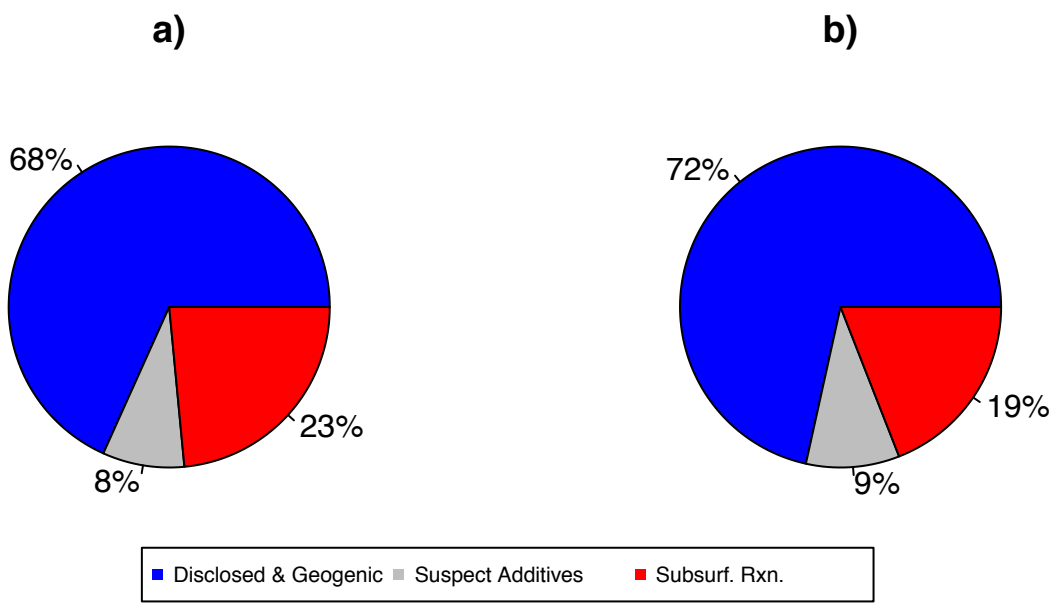

Figure S2: Effect of Retention Index Verification filter for more stringent confidence assignments as a function of putative source of compound. (a) All unique TOF-detected compounds with 85% library matching (n = 729). (b) All TOF-detected compounds with 850 library matching and retention index verification; n= 404). Blue:

Disclosed additives and geogenic compounds. Gray: suspect additives. Red: subsurface reaction products.

Quantitative results and corrections for potential losses

In a two-component system (i.e., air and water), the fraction of the compound present in the air at equilibrium is given by f_{ia}:

$$f_{ia} = \frac{C_{ia}V_a}{C_{iw}V_w + C_{ia}V_a} \qquad Eq.\ S2$$

which, dividing by the numerator, simplifies to:

$$f_{ia} = \frac{1}{1+\frac{C_{iw}V_w}{C_{ia}V_a}} \qquad EqS3$$

or equivalently:

$$f_{ia} = \frac{1}{1+\frac{V_w}{K_{iaw}V_a}} \qquad Eq.S4$$

where V_w and V_a are the volumes [L] of water and air, respectively; C_{iw} and C_{ia} are the concentrations [mass/L] of a compound, *i*, in water and air, respectively; and K_{iaw} [dimensionless] is the air-water partitioning coefficient (obtained from Schwarzenbach et al., 2003)[3]. Here, we estimated that the 250-mL samples containers contained up to 40% headspace.

Note that one could expect some losses of hydrophobic organic chemicals to the HDPE to have occurred also. However, because equilibration with the HDPE will take over two weeks to occur (even for the smaller analytes), performing a similar equilibrium partitioning calculation would be misleading (i.e., it shows that all of the analytes would be absorbed by the PE).

Table S2. Potential losses to the air phase for compounds that have reached equilibrium in an HDPE container that contains headspace. Here, dehp = diethylhexyl phthalate.

Compund	-log (K_{iaw})	f_{ia}	f_{iw}
octane	-2.07	0.987	0.013
octadecane	-0.09	0.451	0.549
tce	0.31	0.246	0.754
benzene	0.65	0.130	0.870
1,2,4-trimethyl benzene	0.65	0.130	0.870
1,4-dichlorobenzene	1.04	0.057	0.943
ethylbenzene	2.80	0.001	0.999
cumene (isopropyl benzene)	3.33	0.000	1.000
m-xylene	2.82	0.001	0.999
p-xylene	2.77	0.001	0.999
toluene	2.22	0.004	0.996
naphthalene	1.74	0.012	0.988
pyrene	3.32	0.000	1.000
phenol	4.59	0.000	1.000
dehp	1.98	0.007	0.993
di-n-butyl phthalate	4.31	0.000	1.000

Note that the values presented here could be used to correct the data presented in Table S3, which shows the uncorrected, measured values.

Table S3. Quantitative outcome of volatile organic compound analysis. Analysis performed using a modified EPA Method 624 (see page S2). Italicized values are below the limit of quantification, but above the limit of detection. Sample names (A-F) correspond to those used in Table S1 and Table 1 in the main text.

Target Analyte	LOQ	Sample Name					
	(µg/L)	A	B	C	D	E	F
1,1,1,2 - Tetrachloroethane	0.4						
1,1,1-Trichloroethane	4						
1,1,2,2-Tetrachloroethane	0.4						
1,1,2-Trichloroethane	2						
1,1-Dichloroethane	2						
1,1-Dichloroethene	2						
1,1-Dichloropropene	4						
1,2,3-Trichlorobenzene	2						
1,2,3-Trichloropropane	10						
1,2,4-Trichlorobenzene	1						
1,2,4-Trimethylbenzene	1		26.8 ± 1.8		0.9 ± 1.1		
1,2-Dibromo-3-chloropropane	20						
1,2-Dibromoethane (EDB)	4						
1,2-Dichlorobenzene	1						
1,2-Dichloroethane	0.8						
1,2-Dichloropropane	1						
1,3-Dichlorobenzene	1						
1,3-Dichloropropane	2						
1,4-Dichlorobenzene	0.4						4.3 ± 0.4
2,2-Dichloropropane	4						
2-Chlorotoluene	0.4						
4-Chlorotoluene	0.4						
4-Isopropyltolune (p-Cymene	1						
Benzene	0.8	*0.3 ± 0.1*			*0.1 ± 0.1*		
Bromobenzene	0.4						
Bromochloromethane	4						
Bromodichloromethane	10						
Bromoform	0.4						
Carbontetrachloride	40						
Chlorobenzene	0.8						
Chloroform	10						
cis-1,2-Dichloroethene	4						
cis-1,3-Dichloropropene	2						
Dibromochloromethane	10						
Dibromomethane	10						
Ethylbenzene	0.8		7.3 ± 0.5				
Hexachlorobutadiene	10						
Isopropylbenzene (Cumene)	2		8.6 ± 0.8				
Methylene Chloride	2						
m-Xylene, p-Xylene	0.4		2.6 ± 0.1				
Naphthalene	1						
n-Butylbenzene	0.4						
n-Propylbenzene	4						
tert-Butylbenzene	1						
Tetrachloroethene	4						
Toluene	0.4		6.2 ± 0.2				
trans-1,2-Dichloroethene	2						
trans-1,3-Dichloropropene	4						
Trichloroethene	4						
sum GRO [ug/L]		5.0 ± 0.02	9.0 ± 0.01	4.1 ± 7.2	2.3 ± 2.6	1.0 ± 0.01	3.8 ± 0.3
sum DRO [mg/L] of LLE extracts		5.9 ± 1.8	13.8 ± 5.6	0.5 ± 0.1	0.3 ± 0.1	1.8 ± 1.0	1.9 ± 0.2

Hopane biomarkers

Biomarker Ratio	Sample A	Sample B
Ts/Tm	1.00	0.88
Ts/(Ts+Tm)	0.50	0.47
HH(S)/HH(S+R)	0.62	0.57
2HH(S)/2HH(S+R)		0.58
Ts/H	0.12	0.15
Tm/H	0.12	0.17
NH/H	0.74	0.90
HH(S)/H	0.10	0.47
HH(R)/H	0.06	0.35
2HH(S)/H		0.28
2HH(R)/H		0.20

Ts = 18a(H)-22,29,30-Trinorneohopane
Tm = 17a(H)-22,29,30-Trinorhopane
HH(S) = 17a(H),21B(H)-22S-Homohopane
HH(R) = 17a(H),21B(H)-22R-Homohopane
H = 17a(H),21B(H)-Hopane
NH = 17a(H),21B(H)-30-Norhopane
2HH(S) = 17a(H),21B(H)-22S-Bishomohopane
2HH(R) = 17B(H),21a(H)-22R-Bishomohopane

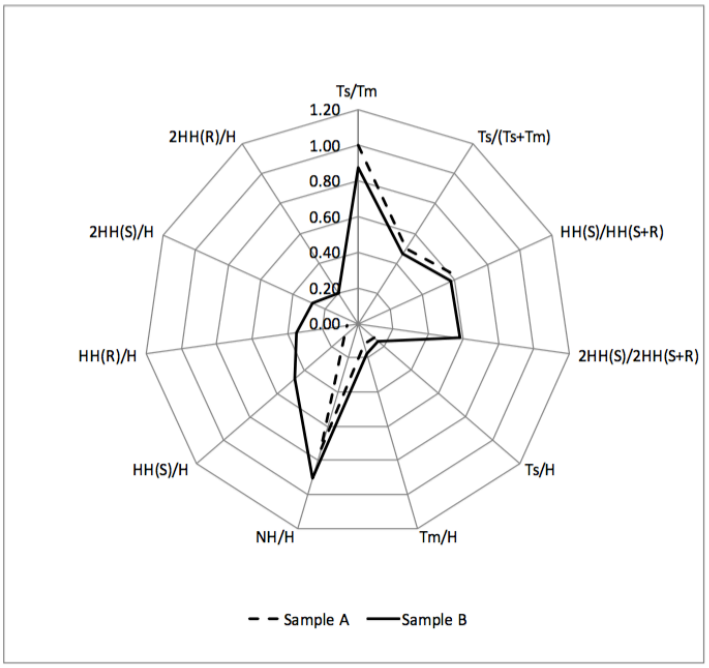

Figure S3. Hopane biomarker patterns and their representative ratios calculated from GCxGC-TOF-MS abundances. Note that the radar plot shows similar character between Sample A and Sample B, and the Ts/Tm ratio suggests the samples are of similar geologic age.

Toxicology and water treatment: Implications

In terms of toxicology and water treatment, the following can be stated: (1) Alcohols and carboxylic acids can be assumed to degrade quickly with exception of phenolic compounds: alkyl phenols are toxic and endocrine disrupting [4, 5] degradation product of alkylphenol polyethoxylates[6]. (2) Phthalates are non- to moderately persistent but may be problematic due to their sorption to soils with consequent partitioning into water[7]. Dibutyl phthalate, which was detected in two samples, is listed on the 2005 Priority List of Hazardous Substances for the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA)[8]. (3) It is precarious that a nitrile serving as a radical initiator could still be detected because it entails the risk of ongoing and unwanted reactivity, leading to further halogenated compound formation. (4) Halogenated hydrocarbons are much more toxic than their parent compounds[9], particularly bromo-and chloroacetones are toxic, irritating gases, which exhibit their effects probably by alkylation of sulfhydryl (SH) -groups of enzymes[10]. Dihalomethanes are mutagenic and reactive[11], dichloromethane is even a suspect human carcinogen[12,13]. One may presume that the general concentrations of iodoalkanes in UNGD wastewaters are very low up to not detectable. However, due to the substances' adverse health effects and low level of scientific examination so far, their occurrence should be investigated more in detail in future studies. (5) UNGD wastewater treatment that is often done by centralized waste treatment facilities (CWTF) only[14], bears the risk of compound survival, hence reaching rivers via effluent. Therefore, aerobic degradation should be implemented additionally, as it is necessary to cope with various organic compounds and to reduce environmental exposure scenarios.

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Table S1 appears on the following pages.

Table S1: Full list of mass spectral library matching-derived tentative identifications and putative compound origins. In columns labeled Sample A-F, an entry corresponds to detection in the respective sample. Y (yes) or N (no) indicates whether a positive confidence assignment could be made based on estimated (est) or experimental (exp) Retention Index (RI) data from the NIST Database. Y' or N' indicates whether a positive confidence assignment could be made based on T (theoretical) or E (experimental) Boiling Points (BP). An entry of "NA" represents a detection without available retention index or boiling point information. Note that some redundancies exist due to the library search software assigning different synonymous names to identical compounds (e.g. "eicosane" and 'n-C20").

Compound Name	CAS RN	1D Retention (sec)	1D RI	NIST RI	RI Type	BP (°C)	BP Type	Disclosure	Compound Source	Sample Name A	B	C	D	E	F
Alcohols										Confidence Assignment (RI BP)					
(2,4,6-Trimethylcyclohexyl) methanol		5010	NA	NA		216	T	implicit	Suspect Frack	-	-	-	-	-	(- N')
1-Decanol	112-30-1	3740	1208.33	1256	exp	231	E	explicit	Frack	(Y Y')	(Y Y')	-	-	(Y Y')	-
1-Dodecanol, 3,7,11-trimethyl-	6750-34-1	4360	1340.00	1563	est	279.2	T	implicit	Suspect Frack	(Y Y')	-	(Y Y')	-	-	(N N')
1-Hexanol	111-27-3	1490	811.67	854	exp	157.6	E	explicit	Frack	-	(Y N')	-	-	-	-
1-Hexanol, 2-ethyl-	104-76-7	2440	970.00	1016	exp	185	E	explicit	Frack	(Y N')	(Y N')	(Y N')	-	-	-
1-Nonanol	143-08-8	3240	1109.80	1157	exp	213.3	E	implicit	Suspect Frack	-	(Y N')	-	-	-	-
1-Octanol	68603-15-6	2690	1012.28	1057	exp	195.1	E	explicit	Frack	(Y N')	(Y N')	-	-	-	-
1-Octanol, 2-methyl-	818-81-5	4160	1295.83	1119	exp	196.6	T	implicit	Suspect Frack	(N N')	-	-	-	-	-
1-Octanol, 3,7-dimethyl-	106-21-8	3340	1129.41	1182	exp	213	E	implicit	Suspect Frack	-	(Y Y')	-	-	-	-
1-Penten-3-ol	616-25-1	4260	1317.78	668	exp	115	E	implicit	Suspect Frack	(N N')	-	-	-	-	-
1-Tridecanol	112-70-9	4120	1287.50	1571	exp	272.1	T	explicit	Frack	(N N')	(N N')	-	-	-	(N N'), (Y Y')
1-Tridecyn-4-ol		5370	1584.62	1473	est	297.4	T	implicit	Suspect Frack	-	-	-	-	-	(N Y')
11-Hexadecyn-1-ol	65686-49-9	5100	1515.38	1872	est	340.1	T	implicit	Suspect Frack	-	(N N')	-	-	-	-
2-Butanol, 2,3-dimethyl-	594-60-5	2050	905.00	716	exp	118.4	E	implicit	Suspect Frack	(N N')	-	(N N')	-	(N N')	(N N')
2-Hexanol, 2-methyl-	625-23-0	2460	973.33	820	exp	143	E	implicit	Suspect Frack	-	-	(N N')	-	-	-
2-Methyl-1-undecanol	10522-26-6	4440	1357.78	1422	exp	245.5	T	implicit	Suspect Frack	-	-	-	-	-	(Y Y')
2-Pentanol, 2,3-dimethyl-	4911-70-0	2490	978.33	745	est	138.3	T	implicit	Suspect Frack	-	-	(N N')	-	-	-
2-Pentanol, 4-methyl-	108-11-2	2420	966.67	752	exp	131.6	E	implicit	Suspect Frack	(N N')	-	-	-	-	-
2-Propyl-1-pentanol	58175-57-8	2730	1019.30	1053	exp	179.2	T	implicit	Suspect Frack	-	-	-	(Y Y')	-	-
2_, 4a_, 8a_-Decahydro-2-naphthalenol		4080	1279.17	1289	est	NA		implicit	Suspect Frack	-	(Y -)	-	-	-	-
3-Hexanol, 2,4-dimethyl-	13432-25-2	2250	938.33	851	est	163.5	T	implicit	Suspect Frack	-	-	-	-	(Y Y')	-
3-Hexanol, 5-methyl-	623-55-2	2050	905.00	838	exp	152.7	T	implicit	Suspect Frack	-	-	-	(Y Y')	-	-
3-Octanol	589-98-0	2270	941.67	984	exp	171	E	implicit	Suspect Frack	-	(Y N')	-	-	-	-
3-Pentanol	584-02-1	1320	92.96	685	exp	114	E	implicit	Suspect Frack	-	-	(N Y')	-	(N Y')	-
3-Pentanol, 2-methyl-	565-67-3	1580	826.67	758	exp	126.5	E	implicit	Suspect Frack	-	(Y Y')	-	-	-	-
3-Pentanol, 3-ethyl-	597-49-9	2310	948.33	853	exp	142	E	implicit	Suspect Frack	-	-	(Y N')	-	-	-
3-Penten-1-ol, 2,2,4-trimethyl-	5842-53-5	1960	890.00	960	est	114	E	implicit	Suspect Frack	-	(Y N')	(Y N')	-	-	-
4-Penten-2-ol	625-31-0	1430	801.67	675	exp	116	E	implicit	Suspect Frack	-	-	-	-	(N Y')	-
5-Methyl-1-hepten-4-ol	99328-46-8	2330	951.67	905	est	172.7	T	implicit	Subsurf. Rxn.	(Y Y')	-	(Y Y')	-	(Y Y')	-
5-Nonadecen-1-ol		4260	1317.78	2161	est	384.6	T	implicit	Subsurf. Rxn.	-	(N N')	-	-	-	-
9,12-Octadecadien-1-ol, (Z,Z)-	506-43-4	6920	2038.71	2069	est	374	T	implicit	Subsurf. Rxn.	-	(Y N')	-	-	-	-
Benzyl Alcohol	100-51-6	2400	963.33	1012	exp	205.3	E	no	Suspect Frack	-	(Y Y')	-	-	(Y Y')	-
cis-9-Tetradecen-1-ol	35153-15-2	5160	1530.77	1655	exp	307.1	T	implicit	Subsurf. Rxn.	-	(N N')	-	-	-	-
Cyclododecanemethanol	1892-12-2	4700	NA	NA		298.7	T	implicit	Subsurf. Rxn.	(- N')	(- N')	-	-	-	-
Cycloheptanemethanol	1131587-94-4	4040	1270.83	1143	est	215.1	T	implicit	Subsurf. Rxn.	-	(N N')	-	-	-	-
Cyclohexanemethanol	100-49-2	4040	1270.83	1023	est	183	E	implicit	Subsurf. Rxn.	-	-	-	-	-	(N N')
Cyclohexanepropanol-	1124-63-6	4000	1262.50	1222	est	218	T	implicit	Subsurf. Rxn.	(Y Y')	-	-	-	-	-
Cyclopentane, 1-hydroxymethyl-1,3-dimethyl-		2830	1036.84	1038	est	173.7	T	implicit	Subsurf. Rxn.	(N N')	(Y Y'), (N N')	(N N')	-	-	(N N')
DL-2,3-Butanediol	6982-25-8	1850	871.67	743	est	183.5	E	no	Suspect Frack	(Y N')	-	(N N')	-	-	-
Dodeca-1,6-dien-12-ol, 6,10-dimethyl-		6290	1839.39	1567	est	292.5	T	implicit	Subsurf. Rxn.	-	(N N')	-	-	-	-
Ethanol, 2-butoxy-	111-76-2	1680	843.33	890	exp	168.4	E	explicit	Frack	-	-	(Y N')	-	-	-
Heptanol	53535-33-4	2110	915.00	953	exp	175.5	E	implicit	Suspect Frack	-	(Y N')	-	-	-	-
Hexadecen-1-ol, trans-9-	64437-47-4	4790	1439.02	1862	est	340	T	implicit	Subsurf. Rxn.	(N N')	-	-	-	-	-
Isopropyl Alcohol	67-63-0	1360	790.00	489	exp	82.5	E	explicit	Frack	-	(N N')	(N N')	-	(N N')	-
Phenol, 2-ethyl-6-methyl-	1687-64-5	3540	1168.63	1227	est	232.4	E	no	Suspect Frack	-	(Y N')	-	-	-	-
Phenol, 3,5-bis(1,1-dimethylethyl)-	1138-52-9	4760	1431.71	1555	est	276.7	T	no	Suspect Frack	-	(N N')	-	-	-	-
Phenol, 4-(1,1,3,3-tetramethylbutyl)-	140-66-9	5500	1618.42	1601	exp	282.3	T	no	Suspect Frack	-	(Y Y')	-	-	-	-
Phenol, 4-methyl-	106-44-5	2670	1008.77	1052	exp	201.9	E	no	Suspect Frack	-	(Y N')	-	-	-	-
Phenol, p-tert-butyl-	98-54-4	3780	1216.67	1261	exp	237	E	no	Suspect Frack	-	(Y N')	-	-	-	-

Compound Name	CAS RN	1D Retention (sec)	1D RI	NIST RI	RI Type	BP (°C)	BP Type	Disclosure	Compound Source	Sample Name A	B	C	D	E	F
Alkanes										Confidence Assignment (RI BP)					
(2-Methylbutyl)cyclohexane	54105-77-0	2880	1045.61	1114	est	197.2	T	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
1-Cyclohexyl-1-(4-methylcyclohexyl)ethane	1161-11-1_	6540	NA	NA		277.9	T	implicit	Frack/Geogenic	-	(- N')	-	-	-	-
1-Methyl-3-ethyladamantane	1687-34-9	3950	1252.08	1127	est	220.9	T	implicit	Frack/Geogenic	-	(N Y')	-	-	-	-
1-Methyl-4-(1-methylethyl)-cyclohexane	99-82-1	4870	1458.54	978	exp	168	E	implicit	Frack/Geogenic	(N N')	-	-	-	-	(N N')
1-Methylbicyclo[3.2.1]octane		4560	1384.44	935	est	148.4	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1,1,6,6-Tetramethylspiro[4.4]nonane		3600	1180.39	1263	est	220	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
1,1'-Bicycloheptyl	23183-11-1	4390	1346.67	1581	est	273.7	T	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	(N N')
1,1'-Bicyclohexyl	92-51-3	3920	1245.83	1313	exp	227	E	implicit	Frack/Geogenic	(Y Y')	(Y Y')	-	-	-	-
1,1'-Bicyclohexyl, 2-ethyl-, cis-	50991-12-3	4640	1402.44	1502	est	264.1	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
1,1'-Bicyclohexyl, 2-ethyl-, trans-	50991-13-4	4640	1402.44	1502	est	264.1	T	implicit	Frack/Geogenic	(Y Y')	(Y Y')	-	-	-	-
1,1'-Bicyclohexyl, 2-methyl-, cis-	50991-08-7	3890	1239.58	1402	est	245	T	implicit	Frack/Geogenic	(N Y'), (Y Y')	(N N'), (Y Y')	-	-	-	(N Y'), (Y Y')
1,1'-Bicyclohexyl, 2-methyl-, trans-	50991-09-8	4150	1293.75	1402	est	245	T	implicit	Frack/Geogenic	(N Y'), (Y Y')	(N Y'), (Y N')	-	-	-	(Y Y')
1,1'-Bicyclohexyl, 2-propyl-, trans-	54934-89-3	4290	1324.44	1601	est	282.3	T	implicit	Frack/Geogenic	(N N')	-	-	-	-	-
1,1'-Bicyclohexyl, 4-methyl-4'-propyl-		5230	1548.72	1662	est	294	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1,1'-Bicyclohexyl, 4,4'-dimethyl-	54823-98-3	4390	1346.67	1463	est	257.6	T	implicit	Frack/Geogenic	(N Y')	(N Y')	-	-	-	(N Y')
1,1'-Bicyclooctyl	6708-17-4	4670	1409.76	1821	est	312	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1,3-Dimethyl-(3,7-dimethyloctyl)cyclohexane		8940	2818.18	1682	est	309.6	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1,3,4-Trimethyladamantane		3780	1216.67	1089	est	214.1	T	implicit	Frack/Geogenic	-	(N Y')	-	-	-	-
1,3,5-Trimethyladamantane	707-35-7	3360	1133.33	1160	exp	207.9	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
1,7-Dimethyl-4-(1-methylethyl)cyclodecane	645-10-3	3830	1227.08	1517	est	270.4	T	implicit	Frack/Geogenic	(N N'), (Y Y')	(N N'), (Y Y')	(N N'), (Y Y')	-	-	(N N')
17a(H)-22,29,30-Trinorhopane		8940	NA	NA		NA		implicit	Frack/Geogenic	-	(- -)	-	-	-	-
17a(H),21B(H)-30-Norhopane		9250	NA	NA		NA		implicit	Frack/Geogenic	-	(- -)	-	-	-	-
1H-Fluorene, dodecahydro-		4010	1264.58	1455	exp	253.5	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
2-Methylbicyclo[3.2.1]octane	766-70-1	4200	1304.44	923	est	156	T	implicit	Frack/Geogenic	(N N')	-	-	-	-	-
2-methylheptadecane (Chiron)	1560-89-0	5810	1700.00	1766	exp	304.9	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
3-methylheptadecane (Chiron)	6418-44-6	5830	1705.71	1774	exp	313.4	T	implicit	Frack/Geogenic	(Y Y')	(N N')	-	-	-	-
4,8-dimethyl-1-cyclohexane (Chiron AS 0827.17 C17H34 mw 238)		4450	NA	NA		NA		implicit	Frack/Geogenic	(- -)	(- -)	(- -)	-	-	(- -)
9-Methyltetracyclo[7.3.1.0(2.7).1(7.11)]tetradecane		4780	1436.59	1348	est	280.5	T	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Adamantane	281-23-2	3880	1237.50	1120	exp	187.1	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Adamantane, 1,3-dimethyl-	702-79-4	2970	1061.40	1157	exp	201	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
alkylcyclohexane (ChC07 mw 182)	5617-41-4	4110	NA	NA		NA		implicit	Frack/Geogenic	(- -)	(- -)	-	-	(- -)	(- -)
alkylcyclohexane (ChC08 mw 196)	1795-15-9	4570	NA	NA		NA		implicit	Frack/Geogenic	-	(- -)	-	-	-	-
alkylcyclohexane (ChC09 mw 210)		4650	NA	NA		NA		implicit	Frack/Geogenic	-	(- -)	-	-	-	-
alkylcyclohexane (ChC18 mw 336)		5280	NA	NA		NA		implicit	Frack/Geogenic	(- -)	-	-	-	-	-
alkylcyclopentane (acp C12 C17H34 mw 238)	5634-30-0	5450	NA	NA		NA		implicit	Frack/Geogenic	-	(- -)	-	-	-	-
Alkylcyclopentane (CpC13 mw 252)	6006-34-4	5060	NA	NA		NA		implicit	Frack/Geogenic	-	(- -)	-	-	-	-
Benzocyclodecene, tetradecahydro-		4450	1360.00	1581	est	277	T	implicit	Subsurf. Rxn.	-	(N N')	-	-	-	-
Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-	473-55-2	5440	1602.63	1002	exp	169	E	implicit	Frack/Geogenic	(N N')	-	-	-	-	(N N')
Bicyclo[4.1.0]heptane, 3-methyl-7-pentyl-		3680	1196.08	1261	est	233.2	T	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-, [1S-(1_,3_,6_)]-		4890	1463.41	937	est	NA		implicit	Frack/Geogenic	(N -)	-	-	-	-	-
Bicyclo[4.1.0]heptane, 7-pentyl-	41977-45-1	3630	1186.27	1200	est	219.7	T	implicit	Frack/Geogenic	(Y Y')	-	-	-	-	-
Butane, 2,2-dimethyl-	75-83-2	3230	1107.84	537	exp	49.7	E	implicit	Frack/Geogenic	-	-	(N N')	-	-	-
C14 Isoprenoid Alkane		3820	NA	NA		NA		explicit	Frack/Geogenic	-	(- -)	-	-	(- -)	(- -)
C15 Isoprenoid Alkane (Farnesane)	3891-98-3	4240	NA	NA		249.1		implicit	Frack/Geogenic	-	(- Y')	(- Y')	(- Y')	-	(- N')
C16 Isoprenoid Alkane		3600	NA	NA		NA	check	implicit	Frack/Geogenic	(- -)	(- -)	(- -)	(- -)	(- -)	(- -)
C18 Isoprenoid Alkane (Norpristane)	3892-00-0	4020	NA	NA		298.2	T	implicit	Frack/Geogenic	(- N')	-	(- N')	(- Y')	(- Y')	(- Y')
C19 Isoprenoid Alkane (Pristane)	1921-70-6	5610	NA	NA		296	E	implicit	Frack/Geogenic	(- Y')	-	(- Y')	(- Y')	(- Y')	(- Y')
C20 Isoprenoid Alkane (Phytane)	638-36-8	5050	NA	NA		322	T	implicit	Frack/Geogenic	(- N')	(- N')	(- Y')	-	-	(- Y')
C21 Isoprenoid Alkane		3780	NA	NA		NA		implicit	Frack/Geogenic	(- -)	(- -)	(- -)	-	-	(- -)
C29-Ts		9240	NA	NA		NA		explicit	Frack/Geogenic	(- -)	-	-	-	-	-
cis-anti-trans-Tricyclo[7.3.0.0(2,6)]dodecane		4300	1326.67	1243	est	232.4	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
cis-Decalin, 2-syn-methyl-	14398-71-1	2840	1038.60	1159	exp	204.6	T	implicit	Frack/Geogenic	-	(N N'), (Y N')	-	-	-	-
cis, cis-3-Ethylbicyclo[4.4.0]decane	1618-23-1	3720	1204.17	1262	est	225.4	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-

Compound Name	CAS RN	1D Retention (sec)	1D RI	NIST RI	RI Type	BP (°C)	BP Type	Disclosure	Compound Source	Sample Name A	B	C	D	E	F
Alkanes cont.										Confidence Assignment (RI BP)					
cis,cis,cis-1-Isobutyl-2,5-dimethylcyclohexane		2990	1064.91	1137	est	205.8	T	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Cyclododecane	294-62-2	3640	1188.24	1145	exp	247	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Cyclohexadecane	295-65-8	5180	1535.90	1918	est	318.7	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Cyclohexane, (1-methylbutyl)-	61208-94-4	2900	1049.12	1114	est	154.8	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Cyclohexane, (1-methylethyl)-	696-29-7	5390	1589.74	920	est	154.8	E	implicit	Frack/Geogenic	-	(N N')	-	-	-	(N N')
Cyclohexane, (1-methylpropyl)-		4000	1262.50	1018	exp	179.3	T	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	-
Cyclohexane, (1,3-dimethylbutyl)-		3510	1162.75	1149	est	212.8	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Cyclohexane, (2-methylpropyl)-	1678-98-4	3470	1154.90	1005	exp	171.3	E	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	(N N')
Cyclohexane, (3-methylpentyl)-	61142-38-9	3240	1109.80	1213	est	218.1	T	implicit	Frack/Geogenic	(N N')	(N N'), (Y Y')	-	-	-	(Y Y')
Cyclohexane, (cyclopentylmethyl)-	4431-89-4	3790	1218.75	1321	est	231.5	T	implicit	Frack/Geogenic	-	(N Y')	-	-	-	-
Cyclohexane, [6-cyclopentyl-3-(3-cyclopentylpropyl)hexyl]-	55401-72-4	9750	3210.53	2592	est	444.9	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Cyclohexane, 1-(1,5-dimethylhexyl)-4-methyl-	29799-19-7	4520	1375.56	1458	exp	265.3	T	implicit	Frack/Geogenic	-	-	-	-	-	(Y N')
Cyclohexane, 1-(cyclohexylmethyl)-3-methyl-, trans-	54823-95-9	4270	1320.00	1502	est	264.9	T	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	-
Cyclohexane, 1-(cyclohexylmethyl)-4-methyl-, cis-	54823-97-1	4550	1382.22	1502	est	264.9	T	implicit	Frack/Geogenic	(Y N')	(N Y')	-	-	-	-
Cyclohexane, 1-ethyl-1-methyl-	4926-90-3	3690	1198.04	902	exp	152.2	E	implicit	Frack/Geogenic	(N N')	(N N')	(N N')	-	-	(N N')
Cyclohexane, 1-ethyl-1,3-dimethyl-, cis-		2550	988.33	1015	est	162.6	T	implicit	Frack/Geogenic	(N N')	(Y Y'), (N N')	-	-	-	(N N')
Cyclohexane, 1-ethyl-1,3-dimethyl-, trans-		2680	1010.53	1015	est	162.6	T	implicit	Frack/Geogenic	(N N')	(Y Y'), (N N')	(N N')	-	-	(N N')
Cyclohexane, 1-ethyl-1,4-dimethyl-, cis-		3510	1162.75	1015	est	162.6	T	implicit	Frack/Geogenic	(N N')	-	-	-	-	(N N')
Cyclohexane, 1-ethyl-1,4-dimethyl-, trans-		3950	1252.08	1015	est	162.6	T	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	-
Cyclohexane, 1-ethyl-2-propyl-	62238-33-9	2750	1022.81	1140	est	196.3	T	implicit	Frack/Geogenic	-	(N N'), (Y Y')	-	-	-	-
Cyclohexane, 1-isopropyl-1-methyl-	16580-26-0	2850	1040.35	989	est	163.5	T	implicit	Frack/Geogenic	(N N')	(Y N'), (N N')	(N N')	-	-	-
Cyclohexane, 1-isopropyl-3-methyl-, trans-	16580-24-8	2780	NA	NA		166.5	E	implicit	Frack/Geogenic	-	(- Y')	-	-	(- N')	-
Cyclohexane, 1-methyl-2-pentyl-	54411-01-7	3390	1139.22	1239	est	216.9	T	implicit	Frack/Geogenic	(Y Y'), (N N')	(Y Y'), (N N')	(N N')	-	-	(N N')
Cyclohexane, 1-methyl-2-propyl-	4291-79-6	3020	1070.18	991	exp	176	E	implicit	Frack/Geogenic	(N N')	(Y Y'), (N N')	-	-	-	(N N')
Cyclohexane, 1-methyl-3-(1-methylethyl)-	16580-24-8	3440	1149.02	976	est	168.2	T	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	(N N')
Cyclohexane, 1-methyl-3-pentyl-		3370	1135.29	1239	est	216.9	T	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	-
Cyclohexane, 1-methyl-3-propyl-	4291-80-9	5620	1650.00	1040	est	164.5	E	implicit	Frack/Geogenic	(N N')	-	(N N')	-	-	(N N')
Cyclohexane, 1-methyl-4-(1-methylbutyl)-	54411-00-6	3180	1098.25	1175	est	211.6	T	implicit	Frack/Geogenic	(Y Y'), (N N')	(Y N'), (N N')	-	-	-	(N N')
Cyclohexane, 1-methyl-4-(1-methylethyl)-, cis-	6069-98-3	4340	1335.56	993	exp	172	E	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	(N N')
Cyclohexane, 1-methyl-4-(1-methylethyl)-, trans-	1678-82-6	5580	1639.47	974	exp	170.6	E	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	-
Cyclohexane, 1,1,2,3-tetramethyl-	6783-92-2	4760	1431.71	976	est	155.8	T	implicit	Frack/Geogenic	-	-	-	-	-	(N N')
Cyclohexane, 1,1,3-trimethyl-2-(3-methylpentyl)-	54965-05-8	4710	1419.51	1409	est	255.3	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Cyclohexane, 1,1,4,4-tetramethyl-		4010	1264.58	989	est	151.3	T	implicit	Frack/Geogenic	(N N')	-	-	-	-	(N N')
Cyclohexane, 1,1'-(1-methyl-1,3-propanediyl)bis-	41851-35-8	5300	1566.67	1675	est	302.3	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Cyclohexane, 1,1'-(1,2-dimethyl-1,2-ethanediyl)bis-	74663-71-1	3710	1202.08	1610	est	297.3	T	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	-
Cyclohexane, 1,1'-(1,3-propanediyl)bis-	3178-24-3	4960	1480.49	1639	est	291.5	E	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Cyclohexane, 1,1'-(1,4-butanediyl)bis-	6165-44-2	5610	1647.37	1715	exp	305	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Cyclohexane, 1,1'-methylenebis-	3178-23-2	4040	1270.83	1402	exp	252.7	T	implicit	Frack/Geogenic	(N N'), (Y N')	(N N'), (Y N')	-	-	-	(Y N')
Cyclohexane, 1,2-diethyl-, cis-	3642-13-5_	4160	1295.83	1040	est	174.3	T	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	-
Cyclohexane, 1,2-dimethyl-3-pentyl-4-propyl-	62376-17-4	4750	1429.27	1560	est	281.9	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Cyclohexane, 1,4-dimethyl-2-(2-methylpropyl)-, (1_,2ö,5_)-		3230	1107.84	1137	est	NA		implicit	Frack/Geogenic	-	(Y -)	-	-	-	-
Cyclohexane, 1,5-diisopropyl-2,3-dimethyl-		4140	1291.67	1233	est	235.4	T	implicit	Frack/Geogenic	(Y Y')	-	-	-	-	-
Cyclohexane, 2-butyl-1,1,3-trimethyl-	54676-39-0	3560	1172.55	1274	est	221	T	implicit	Frack/Geogenic	-	(N Y'), (Y Y')	-	-	-	-
Cyclohexane, 2,4-diethyl-1-methyl-	61142-70-9	3730	1206.25	1114	est	189.8	T	implicit	Frack/Geogenic	(Y N'), (N N')	(Y N')	-	-	(N N')	(N N')
Cyclohexane, 3-ethyl-5-methyl-1-propyl-		3130	1089.47	1201	est	211	T	implicit	Frack/Geogenic	(Y N')	(N N'), (Y Y')	-	-	-	(Y Y')
Cyclohexane, butyl-	1678-93-9	2520	983.33	1029	exp	180.9	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Cyclohexane, decyl-	1795-16-0	5400	1592.31	1649	exp	299	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	(N N')	-
Cyclohexane, heptyl-	5617-41-4	3620	1184.31	1340	exp	244	E	implicit	Frack/Geogenic	-	-	-	-	(N N')	-
Cyclohexane, hexyl-	4292-75-5	3620	1184.31	1233	exp	224	E	implicit	Frack/Geogenic	(Y Y')	(Y Y'), (N N')	-	-	-	-
Cyclohexane, nonyl-		4570	1386.67	1545	exp	282.6	T	implicit	Frack/Geogenic	-	-	-	-	(N N')	-
Cyclohexane, octyl-	1795-15-9	4560	1384.44	1440	exp	264	E	implicit	Frack/Geogenic	(Y Y'), (N N')	-	(Y Y'), (N N')	-	-	(Y Y')
Cyclohexane, pentyl-	4292-92-6	3090	1082.46	1130	exp	203.7	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Cyclohexane, undecyl-	54105-66-7	5400	1592.31	1775	est	315.8	T	implicit	Frack/Geogenic	(Y N')	(N N')	-	-	(N N')	-
Cyclohexene, 1-ethyl-	1453-24-3	2700	1014.04	863	exp	137	E	implicit	Frack/Geogenic	-	(N N')	-	-	-	-

Compound Name	CAS RN	1D Retention (sec)	1D RI	NIST RI	RI Type	BP (°C)	BP Type	Disclosure	Compound Source	Sample Name A	B	C	D	E	F
Alkanes cont.										Confidence Assignment (RI BP)					
Cyclohexene, 1-pentyl-	15232-85-6	2930	1054.39	1135	exp	203.6 T		implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Cyclohexene, 4-(4-ethylcyclohexyl)-1-pentyl-		4860	1456.10	1971	exp	345.2 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Cyclohexene,1-heptyl-	15232-86-7	4080	1279.17	1388	est	243.9 T		implicit	Frack/Geogenic	-	(N Y')	-	-	-	-
Cyclohexene,4-butyl-	21524-26-5	2870	1043.86	1046	exp	178.2 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Cyclooctane, (1-methylpropyl)-	16538-89-9	2790	1029.82	1254	est	221.3 T		implicit	Frack/Geogenic	(Y Y'), (N N')	(N N')	-	-	-	(Y N')
Cyclooctane, 1,2-diethyl-	23609-46-3	3500	1160.78	1280	est	220.6 T		implicit	Frack/Geogenic	(Y Y')	(N Y')	-	-	-	-
Cyclooctane, 1,2-dimethyl-	13151-94-5	3470	1154.90	1081	est	177.6 T		implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Cyclooctane, 1,4-dimethyl-, trans-	13151-98-9	3990	1260.42	1081	est	177.6 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Cyclooctane, cyclohexyl-		3750	1210.42	1581	est	273.7 T		implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	(N N')
Cyclooctane, ethyl-	13152-02-8	4550	1382.22	1120	est	184.8 T		implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	-
Cyclooctane, methyl-	1502-38-1	4590	1391.11	1020	est	161.9 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
Cyclopentadecane	295-48-7	4770	1434.15	1799	est	300.1 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
Cyclopentadecanone, 2-methyl-		6850	2016.13	2031	est	329.5 T		implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Cyclopentane, (2-methylbutyl)-	53366-38-4	4410	1351.11	994	est	173.4 T		implicit	Frack/Geogenic	-	-	-	-	-	(N N')
Cyclopentane, (3-methylbutyl)-	1005-68-1	4420	1353.33	994	est	173.4 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
Cyclopentane, 1-butyl-2-ethyl-	72993-32-9	4770	1434.15	1119	est	194.5 T		implicit	Frack/Geogenic	-	-	-	-	-	(N N')
Cyclopentane, 1-butyl-2-propyl-	62199-50-3	4340	1335.56	1219	est	215.4 T		implicit	Frack/Geogenic	(N N')	-	(N N')	-	-	-
Cyclopentane, 1-ethyl-3-methyl-, trans-	2613-65-2	4200	1304.44	786	exp	121 E		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
Cyclopentane, 1-hexyl-3-methyl-	61142-68-5_	2860	1042.11	1219	est	215.2 T		implicit	Frack/Geogenic	(Y Y')	(N N')	(N N')	-	-	(N N')
Cyclopentane, 1-methyl-2-propyl-	3728-57-2	4480	1366.67	883	exp	148.9 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
Cyclopentane, 1-methyl-3-(2-methylpropyl)-	29053-04-1	3850	1231.25	956	est	166.7 T		implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	-
Cyclopentane, 1-pentyl-2-propyl-	62199-51-3	3790	1218.75	1318	est	235.5 T		implicit	Frack/Geogenic	-	(Y N'), (N N')	-	-	-	-
Cyclopentane, 1,1,3-trimethyl-3-(2-methyl-2-propenyl)-	74421-09-3	4200	1304.44	1134	est	189.2 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	(N N')
Cyclopentane, 1,1'-(1,4-butandiyl)bis-	2980-70-3	3840	1229.17	1499	est	268.7 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Cyclopentane, 1,1'-[4-(3-cyclopentylpropyl)-1,7-heptanediyl]bis-	55429-35-1	10330	3522.22	2571	est	443.5 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Cyclopentane, 1,1'-ethylidenebis-	4413-21-2	3510	1162.75	1236	est	223.7 T		implicit	Frack/Geogenic	-	(Y N'), (N N')	-	-	-	-
Cyclopentane, 1,2-dibutyl-	62199-52-4	3920	1245.83	1318	est	235.5 T		implicit	Frack/Geogenic	(Y Y')	-	-	-	-	-
Cyclopentane, 1,2-dimethyl-3-(1-methylethyl)-	489-20-3	3660	1192.16	918	est	159.8 T		implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	(N N')
Cyclopentane, 1,3-dimethyl-2-(1-methylethenyl)-, (1_,2_,3ö)-		4560	1384.44	906	exp	159.8 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Cyclopentane, 2-isopropyl-1,3-dimethyl-	32281-85-9	3510	1162.75	918	est	159.8 T		implicit	Frack/Geogenic	(N N')	(N N')	(N N')	-	-	(N N')
Cyclopentane, heneicosyl-	6703-82-8	6790	1996.77	2649	est	423.2 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Cyclopentane, hexyl-	4457-00-5	3640	1188.24	1136	exp	203 E		implicit	Frack/Geogenic	(Y Y'), (N N')	(N N'), (Y Y')	-	-	-	(N N')
Cyclopentene, 5-hexyl-3,3-dimethyl-		3640	NA	NA		222.5 T		implicit	Frack/Geogenic	(- Y')	(- Y')	-	-	-	-
Cyclopentylcyclohexane	1606-08-2	3360	1133.33	1221	est	215.1 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Cyclopropane, 1-methyl-2-(3-methylpentyl)-	62238-07-7	3400	1141.18	915	est	163 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	(N N')
Cyclopropane, 1,2-dimethyl-, trans-		1100	746.67	482	est	31.7 T		implicit	Frack/Geogenic	-	-	(N N')	-	-	-
Cyclopropane, 1,2-dimethyl-1-pentyl-	62238-04-4	4540	1380.00	953	est	157.2 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
Cyclopropane, nonyl-	74663-85-7	4910	1468.29	1216	est	219.8 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
Cyclotetradecane	295-17-0	4580	1388.89	1679	est	280.9 T		implicit	Frack/Geogenic	(N Y')	(N N')	-	-	-	-
Cycloundecene, 1-methyl-	88828-82-4	3140	1091.23	1391	est	233.1 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Decahydro-4,4,8,9,10-pentamethylnaphthalene	80655-44-3	4260	1317.78	1432	est	248.9 T		implicit	Frack/Geogenic	-	(N Y')	-	-	-	-
Decalin, syn-1-methyl-, cis-	14398-67-5	2910	1050.88	1162	est	210 T		implicit	Frack/Geogenic	-	(N N'), (Y Y')	-	-	-	-
Decane	124-18-5	2360	956.67	1000	exp	173 E		explicit	Frack/Geogenic	(Y Y'), (N N')	(Y Y')	(Y Y')	-	(Y Y')	(Y Y')
Decane, 2-cyclohexyl-	13151-73-0	6040	1765.71	1611	est	293.1 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Decane, 2-methyl-	6975-98-0	4220	1308.89	1065	exp	189.3 E		implicit	Frack/Geogenic	-	(Y Y')	(N N')	-	-	-
Decane, 2,3,5-trimethyl-	62238-11-3	4400	1348.89	1121	est	217.4 T		implicit	Frack/Geogenic	-	-	(N N')	-	-	-
Decane, 2,3,5,8-tetramethyl-	192823-15-7	6030	1762.86	1156	est	230.5 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
Decane, 2,4-dimethyl-	2801-84-5	4150	1293.75	1086	est	204.7 T		implicit	Frack/Geogenic	-	-	(N N')	(N N')	-	-
Decane, 2,5,9-trimethyl-	62108-22-9	5310	1569.23	1121	est	212.2 T		implicit	Frack/Geogenic	-	-	(N N')	-	-	-
Decane, 2,9-dimethyl-	1002-17-1	4680	1412.20	1138	exp	202.4 T		implicit	Frack/Geogenic	-	-	(N N')	-	-	(N N')
Decane, 3-methyl-	13151-34-3	4180	1300.00	1072	exp	188.1 E		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Decane, 3,7-dimethyl-	17312-54-8	3080	1080.70	1133	exp	203 T		implicit	Frack/Geogenic	(Y Y'), (N N')	-	-	-	-	-
Decane, 3,8-dimethyl-	17312-55-9	8570	2658.33	1140	exp	204.6 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
Decane, 5-propyl-	17312-62-8	4590	1391.11	1249	est	218.2 T		implicit	Frack/Geogenic	-	-	-	-	-	(N N')

Compound Name	CAS RN	1D Retention (sec)	1D RI	NIST RI	RI Type	BP (°C)	BP Type	Disclosure	Compound Source	Sample Name A	B	C	D	E	F
Alkanes cont.										Confidence Assignment (RI BP)					
Decane, 6-ethyl-2-methyl-	62108-21-8	4080	1279.17	1185	est	217 T	implicit	Frack/Geogenic		(N N')	-	-	-	-	(Y N'), (N N')
Dia(Ba)C27(R): 13B(H),17a(H)-20R-24-Ethyl-Cholestane		8740	NA	NA		NA	implicit	Frack/Geogenic		-	(- -)	-	-	-	-
Dispiro[4.2.4.2]tetradecane		4300	1326.67	1508	est	284.7 T	implicit	Frack/Geogenic		-	(N N'), (Y N')	-	-	-	-
Dodecane	112-40-3	3450	1150.98	1200	exp	216 E	explicit	Frack/Geogenic		(Y Y')	(Y Y')	-	-	(Y Y')	-
Dodecane, 2-methyl-	1560-97-0	3760	1212.50	1265	exp	227.7 T	implicit	Frack/Geogenic		(N N')	(N N')	-	-	(Y Y')	(Y Y'), (N N')
Dodecane, 2,6,10-trimethyl-	3891-98-3	3760	1212.50	1379	exp	249.1 T	implicit	Frack/Geogenic		(N N'), (Y Y')	(N N')	-	-	(Y Y')	(Y Y')
Dodecane, 2,6,11-trimethyl-	31295-56-4	4470	1364.44	1320	est	247.8 T	implicit	Frack/Geogenic		(N N')	-	(N N')	-	-	(Y Y'), (N N')
Dodecane, 2,7,10-trimethyl-	74645-98-0	4880	1460.98	1320	est	249.1 T	implicit	Frack/Geogenic		-	(N N')	(N N')	-	-	(N N')
Dodecane, 3-methyl-	17312-57-1	3800	1220.83	1271	exp	229.3 T	implicit	Frack/Geogenic		(Y Y')	-	-	(Y Y')	(Y Y')	-
Dodecane, 4-methyl-	6117-97-1	3740	1208.33	1260	exp	227.8 T	implicit	Frack/Geogenic		-	-	-	-	-	(Y Y')
Dodecane, 5-methyl-	17453-93-9	5760	1686.84	1256	exp	226.6 T	implicit	Frack/Geogenic		-	-	-	-	-	(N N')
Dodecane, 6-methyl-	6044-71-9	3710	1202.08	1254	exp	224.8 T	implicit	Frack/Geogenic		-	-	-	-	-	(Y Y')
Eicosane	112-95-8	6260	1830.30	2000	exp	343 E	implicit	Frack/Geogenic		(N N')	(N N')	-	-	-	(N N')
Heptacosane	593-49-7	9440	3055.00	2700	exp	463.8 E	implicit	Frack/Geogenic		-	(N Y')	-	-	-	-
Heptadecane	629-78-7	5570	1636.84	1700	exp	302 E	implicit	Frack/Geogenic		(Y Y')	-	-	(Y Y')	(Y Y')	-
Heptadecane, 2-methyl-	1560-89-0	5440	1602.63	1766	exp	311 E	implicit	Frack/Geogenic		-	-	-	(N N')	-	-
Heptadecane, 2,6-dimethyl-	54105-67-8	4530	1377.78	1782	est	318.1 T	implicit	Frack/Geogenic		-	-	-	-	(N N')	-
Heptadecane, 2,6,10,14-tetramethyl-	18344-37-1	4560	1384.44	1895	exp	356.9 T	implicit	Frack/Geogenic		-	-	(N N')	-	-	-
Heptadecane, 4-methyl-	26429-11-8	5780	1692.11	1760	exp	312.6 T	implicit	Frack/Geogenic		(Y Y')	-	-	-	-	-
Heptadecane, 7-methyl-	20959-33-5	5740	1681.58	1745	exp	308.7 T	implicit	Frack/Geogenic		-	(Y Y')	-	-	-	-
Heptadecane, 8-methyl-	13287-23-5	5610	1647.37	1756	exp	306.2 T	implicit	Frack/Geogenic		-	(N Y')	-	-	-	-
Heptane, 2-methyl-	592-27-8	990	728.33	766	exp	117.6 E	implicit	Frack/Geogenic		-	(Y Y')	-	-	-	-
Heptane, 2,3,6-trimethyl-	4032-93-3	2140	920.00	919	exp	156 E	implicit	Frack/Geogenic		-	(Y Y')	-	-	-	-
Heptane, 3-ethyl-5-methylene-		1910	881.67	918	est	161 T	implicit	Frack/Geogenic		-	-	(Y N')	-	-	-
Hexadecane	544-76-3	4110	1285.42	1600	exp	287 E	explicit	Frack/Geogenic		(N N'), (Y Y')	(Y Y'), (N N')	(N N'), (Y Y')	(Y Y')	(Y Y')	(Y Y'), (N N')
Hexadecane, 2-methyl-	1560-92-5	5090	1512.82	1665	exp	291.4 T	implicit	Frack/Geogenic		(Y Y')	(N N'), (Y Y')	-	-	-	-
Hexadecane, 7-methyl-	26730-20-1	5380	1587.18	1647	exp	292.1 T	implicit	Frack/Geogenic		-	(Y Y')	-	-	-	-
Hexane, 2,4-dimethyl-	589-43-5	4810	1443.90	734	exp	109.2 T	implicit	Frack/Geogenic		-	(N N')	-	-	-	-
Hexane, 3,3-dimethyl-	563-16-6	7050	2080.65	741	exp	111.9 E	implicit	Frack/Geogenic		(N N')	-	-	-	-	(N N')
n-C13		3930	1247.92	1300	exp	235 E	explicit	Frack/Geogenic		-	(Y Y')	-	-	-	-
n-C14		4380	1344.44	1400	exp	253 E	explicit	Frack/Geogenic		-	(Y Y')	-	-	-	-
n-C16		4660	1407.32	1600	exp	287 E	explicit	Frack/Geogenic		(N N')	(N N'), (Y Y')	-	-	-	-
n-C18		5540	1628.95	1800	exp	317 E	explicit	Frack/Geogenic		(Y Y')	(N N')	-	-	-	-
n-C19		5310	1569.23	1900	exp	330.5 E	explicit	Frack/Geogenic		(N N')	(N N'), (Y Y')	-	-	-	-
n-C20		6010	1757.14	2000	exp	342.7 E	explicit	Frack/Geogenic		(Y Y')	(N N'), (Y Y')	-	-	-	-
n-C21		6890	2029.03	2100	exp	356.1 T	explicit	Frack/Geogenic		-	-	-	(Y Y')	-	-
n-Nonylcyclohexane		4850	1453.66	1545	exp	282.6 T	implicit	Frack/Geogenic		(Y Y')	(Y N')	-	-	-	(Y Y')
n-Tridecylcyclohexane	6006-33-3	7400	2200.00	1949	exp	345.7 T	implicit	Frack/Geogenic		-	(N N'), (Y N')	-	-	-	-
Nonadecane	629-92-5	6530	1912.90	1900	exp	330.5 E	implicit	Frack/Geogenic		-	(Y Y'), (N N')	-	(Y Y')	-	-
Nonadecane, 2-methyl-	1560-86-7	6460	1890.91	1966	exp	329.7 T	implicit	Frack/Geogenic		-	(Y Y')	-	-	-	-
Nonane	111-84-2	1760	856.67	900	exp	151 E	explicit	Frack/Geogenic		(Y N')	(Y N')	-	-	-	-
Nonane, 2-methyl-	871-83-0	2160	923.33	965	exp	167.1 E	implicit	Frack/Geogenic		-	(Y N')	-	-	-	-
Nonane, 2,6-dimethyl-	17302-28-2	2510	981.67	1026	exp	180.6 T	implicit	Frack/Geogenic		-	(Y Y')	-	-	-	(N N')
Nonane, 3-methyl-		2200	930.00	971	exp	167.9 T	implicit	Frack/Geogenic		-	(Y Y')	-	-	-	-
Nonane, 3-methyl-5-propyl-	31081-18-2	4510	1373.33	1052	exp	213.1 T	implicit	Frack/Geogenic		-	-	(N N')	-	-	(N N')
Nonane, 3,7-dimethyl-	17302-32-8	2600	996.67	1042	exp	183.3 T	implicit	Frack/Geogenic		-	(Y Y')	-	-	-	-
Octadecane	593-45-3	5930	1734.29	1800	exp	317 E	implicit	Frack/Geogenic		-	(Y Y'), (N N')	-	(Y Y')	-	-
Octadecane, 2-methyl-	1560-88-9	6150	1797.14	1864	exp	317.7 T	implicit	Frack/Geogenic		-	(Y Y')	-	-	-	-
Octadecane, 4-methyl-	10544-95-3	6130	1791.43	1860	exp	325.8 T	implicit	Frack/Geogenic		-	(Y Y')	-	-	-	-
Octadecane, 5-methyl-	25117-35-5	6110	1785.71	1853	exp	325.2 T	implicit	Frack/Geogenic		-	(Y Y')	-	-	-	-
Octane	111-65-9	1160	756.70	800	exp	125.5 E	implicit	Frack/Geogenic		(Y N')	(Y N')	-	-	(Y Y')	-
Octane, 2-cyclohexyl-		4050	1272.92	1412	est	256.9 T	implicit	Frack/Geogenic		(N N'), (Y Y')	-	-	-	-	(Y Y')
Octane, 2,2,6-trimethyl-	62016-28-8	2150	921.67	966	est	172.3 T	implicit	Frack/Geogenic		-	-	-	-	(Y N')	-
Octane, 2,3,7-trimethyl-	62016-34-6	3810	1222.92	922	est	179.3 T	implicit	Frack/Geogenic		-	-	(N N')	-	-	-

Compound Name	CAS RN	1D Retention (sec)	1D RI	NIST RI	RI Type	BP (°C)	BP Type	Disclosure	Compound Source	Sample Name A	B	C	D	E	F
Alkanes cont.										Confidence Assignment (RI BP)					
Octane, 2,4,6-trimethyl-	62016-37-9	2830	1036.84	955	exp	172.2	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Octane, 2,6,6-trimethyl-	54166-32-4	5680	1665.79	966	est	176.1	T	implicit	Frack/Geogenic	-	-	(N N')	-	-	-
Octane, 2,7-dimethyl-	1072-16-8	5060	1505.13	929	exp	159.9	E	implicit	Frack/Geogenic	-	-	-	(N N')	-	-
Octane, 3-ethyl-2,7-dimethyl-	62183-55-5	3200	1101.96	1022	est	198.6	T	implicit	Frack/Geogenic	(Y Y'), (N N')	-	-	-	-	-
Octane, 4-bromo-		5120	1520.51	1049	est	190.8	T	implicit	Frack/Geogenic	-	-	(N N')	-	-	-
Octane, 4-ethyl-	15869-86-0	3230	1107.84	956	exp	163.7	E	implicit	Frack/Geogenic	(N N')	-	-	-	-	-
Octane, 4-methyl-	2216-34-4	1540	820.00	865	exp	142.4	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Octane, 6-ethyl-2-methyl-	62016-19-7	2920	1052.63	986	est	181.2	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Pentacyclo[7.3.1.1.(4,12).0(2,7).0(6,11)]tetradecane(diamantan)	2292-79-7	4790	1439.02	1164	est	269.5	T	implicit	Frack/Geogenic	-	(N Y')	-	-	-	-
Pentadecane	629-62-9	4800	1441.46	1500	exp	269.5	E	explicit	Frack/Geogenic	(Y Y')	(Y Y'), (N N')	-	(Y Y')	(Y Y')	(Y Y')
Pentadecane, 2-methyl-	1560-93-6	5060	1505.13	1565	exp	282	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Pentadecane, 2,6,10-trimethyl-	3892-00-0	5180	1535.90	1652	exp	298.2	T	implicit	Frack/Geogenic	-	(N N'), (Y Y')	-	-	-	-
Pentadecane, 3-methyl-	2882-96-4	5080	1510.26	1572	exp	282.7	T	implicit	Frack/Geogenic	-	-	-	-	-	(Y Y')
Pentadecane, 7-methyl-	6165-40-8	6080	1777.14	1548	exp	277.1	T	implicit	Frack/Geogenic	(N N')	-	-	-	-	-
Pentadecane, 8-heptyl-	71005-15-7	9230	2952.38	2144	est	382.8	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Pentane, 2,3,4-trimethyl-	565-75-3	3630	1186.27	690	exp	113.5	E	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Pentane, 3-ethyl-	617-78-7	2020	900.00	686	exp	93.5	E	implicit	Frack/Geogenic	-	-	-	-	-	(N N')
Pentane, 3-ethyl-2,4-dimethyl-	1068-87-7	7610	2277.78	837	est	136.7	E	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Perhydrophenalene, (3a_, 6a_, 9a_, 9bö)-		4140	1291.67	1363	est	NA		implicit	Frack/Geogenic	-	(Y -)	-	-	-	-
Phenanthrene, tetradecahydro-	5743-97-5	4650	1404.88	1539	exp	273.7	T	implicit	Frack/Geogenic	(N N'), (Y Y')	(N N'), (Y Y')	-	-	-	-
Pyrene, hexadecahydro-	2435-85-0	5430	1600.00	1502	est	318.5	T	implicit	Frack/Geogenic	(Y N')	(N N')	-	-	-	-
Tetradecahydro-1-methylphenanthrene		4620	1397.78	1539	exp	284.8	T	implicit	Frack/Geogenic	(Y N')	(N N'), (Y N')	-	-	-	-
Tetradecane	629-59-4	3930	1247.92	1400	exp	253	E	explicit	Frack/Geogenic	(N N'), (Y Y')	(N N'), (Y Y')	-	(Y Y')	(N N'), (Y Y')	(Y Y')
Tetradecane, 2-methyl-	1560-95-8	4650	1404.88	1465	exp	261.6	T	implicit	Frack/Geogenic	(Y Y')	-	-	-	-	(Y Y')
Tetradecane, 3-methyl-	18435-22-8	4530	1377.78	1472	exp	265.1	T	implicit	Frack/Geogenic	(Y Y')	(Y N')	-	-	(Y Y')	(Y Y')
Tetradecane, 4-methyl-	25117-24-2	4230	1311.11	1460	exp	263.8	T	implicit	Frack/Geogenic	-	-	-	-	-	(N N'), (Y Y')
Tetradecane, 5-methyl-	25117-32-2	4610	1395.56	1454	exp	262.8	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	(Y Y')
trans-anti-trans-Tetra-decahydroanthracene	28071-99-0	4700	1417.07	1483	est	273.7	T	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
tricyclic terpane C21H38 mass 290		5550	NA	NA		NA		implicit	Frack/Geogenic	-	(- -)	-	-	-	-
tricyclic terpane C25H46 mass 346		9660	NA	NA		NA		implicit	Frack/Geogenic	-	(- -)	-	-	-	-
tricyclic terpane C26H48b mass 360		9800	NA	NA		NA		implicit	Frack/Geogenic	-	(- -)	-	-	-	-
tricyclic terpane C28H52b mass 388		9420	NA	NA		NA		implicit	Frack/Geogenic	(- -)	-	-	-	-	-
Tricyclo[4.4.1.0(1,6)]undecane		4310	1328.89	1148	est	223.2	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Tricyclo[6.4.0.0(2,7)]dodecane	53485-49-7	3840	1229.17	1344	exp	232.4	T	implicit	Frack/Geogenic	-	(N Y')	-	-	-	-
Tricyclo[7.3.0.0(2,6)]dodecane, trans-anti-trans-		3850	1231.25	1243	est	232.4	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Tridecane	629-50-5	3930	1247.92	1300	exp	234.5	E	explicit	Frack/Geogenic	(Y Y')	(N N')	(N N')	-	(Y Y')	(Y Y')
Tridecane, 2-methyl-	1560-96-9	4220	1308.89	1365	exp	245.2	T	implicit	Frack/Geogenic	(Y Y'), (N N')	(Y Y')	-	-	(Y Y')	(Y Y')
Tridecane, 3-ethyl-	13286-73-2	4660	1407.32	1448	est	265.6	T	implicit	Frack/Geogenic	(Y Y')	-	-	-	-	-
Tridecane, 3-methyl-	6418-41-3	4250	1315.56	1372	exp	248.7	T	implicit	Frack/Geogenic	(N N')	-	(Y Y')	(Y Y')	(Y Y')	(Y Y')
Tridecane, 4-methyl-	26730-12-1	3770	1214.58	1360	exp	247.4	T	implicit	Frack/Geogenic	(N N')	(Y Y')	-	-	-	(Y Y')
Tridecane, 4,8-dimethyl-	55030-62-1	4410	1351.11	1407	exp	256.1	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	(Y Y')	-
Tridecane, 5-methyl-	25117-31-1	4180	1300.00	1354	exp	246.3	T	implicit	Frack/Geogenic	(Y Y')	(Y Y')	-	-	-	-
Tridecane, 6-methyl-	13287-21-3	4170	1297.92	1353	exp	244.6	T	implicit	Frack/Geogenic	-	-	-	-	-	(Y Y')
Undecane	1120-21-4	2930	1054.39	1100	exp	196	E	explicit	Frack/Geogenic	(Y Y'), (N N')	(N N'), (Y Y')	-	-	-	(N N')
Undecane, 2-methyl-	7045-71-8	3270	1115.69	1165	exp	208.9	T	implicit	Frack/Geogenic	(Y Y')	(Y Y')	(N N')	-	-	-
Undecane, 2,4-dimethyl-	17312-80-0	4980	1485.37	1208	exp	220.3	T	implicit	Frack/Geogenic	(N N')	-	(N N')	-	-	-
Undecane, 2,6-dimethyl-	17301-23-4	3520	1164.71	1216	exp	218.9	T	implicit	Frack/Geogenic	-	(Y Y')	(Y Y')	-	(Y Y')	(Y Y')
Undecane, 2,8-dimethyl-	17301-25-6	5680	1665.79	1222	exp	221.8	T	implicit	Frack/Geogenic	-	-	-	-	-	(N N')
Undecane, 2,9-dimethyl-	17301-26-7	3660	1192.16	1234	exp	223.3	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Undecane, 3-methyl-	1002-43-3	3310	1123.53	1172	exp	210.8	T	implicit	Frack/Geogenic	(Y Y')	(N N')	(N N')	-	-	(N N')
Undecane, 3,5-dimethyl-	17312-81-1	4150	1293.75	1209	exp	219.8	T	implicit	Frack/Geogenic	-	-	-	-	-	(Y N')
Undecane, 3,7-dimethyl-	17301-29-0	10330	3522.22	1221	exp	221.8	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Undecane, 3,8-dimethyl-	17301-30-3	7530	2248.15	1228	exp	223	T	implicit	Frack/Geogenic	(N N')	-	-	-	-	-
Undecane, 4-methyl-	2980-69-0	3250	1111.76	1161	exp	209.2	T	implicit	Frack/Geogenic	(Y Y')	-	-	-	-	-

Compound Name	CAS RN	1D Retention (sec)	1D RI	NIST RI	RI Type	BP (°C)	BP Type	Disclosure	Compound Source	Sample Name A	B	C	D	E	F
Alkanes cont.										Confidence Assignment (RI BP)					
Undecane, 4,7-dimethyl-	17301-32-5	4540	1380.00	1207	exp	220.3 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
Undecane, 5-ethyl-	17453-94-0	3660	1192.16	1249	est	223.8 T		implicit	Frack/Geogenic	-	-	(N N')	-	-	(Y Y')
Undecane, 5-methyl-	632-70-8	3230	1107.84	1157	exp	207.9 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Alkenes															
1-Decene	872-05-9	3990	1260.42	987	exp	170.5 E		implicit	Frack/Geogenic	-	-	-	-	-	(N N')
1-Decene, 8-methyl-	61142-79-8	3920	1245.83	1062	exp	183.7 T		implicit	Frack/Geogenic	-	-	-	-	-	(N N')
1-Docosene	1599-67-3	4710	1419.51	2192	exp	364.6 E		implicit	Frack/Geogenic	(N N')	(N N'), (Y Y')	(N N')	-	-	(N N')
1-Heptene, 4-methyl-	13151-05-8	1920	883.33	755	exp	112.8 E		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1-Heptene, 6-methyl-	5026-76-6	4120	1287.50	754	exp	113.2 E		implicit	Frack/Geogenic	-	-	(N N')	-	-	-
1-Hexadecene	629-73-2	4830	1448.78	1590	exp	284.9 E		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1-Hexene, 3,3,5-trimethyl-	13427-43-5	3780	1216.67	757	est	127.1 T		implicit	Frack/Geogenic	-	-	-	-	-	(N N')
1-Hexene, 4,5-dimethyl-	16106-59-5	2020	900.00	747	exp	106.9 T		implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	-
1-Nonadecene	18435-45-5	5930	1734.29	1891	exp	329.0 E		implicit	Frack/Geogenic	-	(N N')	-	(Y Y')	-	-
1-Nonene, 4,6,8-trimethyl-	54410-98-9	4380	1344.44	1012	est	195.7 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1-Octadecyne	629-89-0	4730	1424.39	1808	est	313.0 E		implicit	Frack/Geogenic	-	-	-	-	-	(Y Y')
1-Octene, 3,7-dimethyl-		3590	1178.43	963	exp	156.2 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	(N N')
1-Octene, 4-methyl-	13151-12-7	4170	1297.92	842	est	137.6 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
1-Octene, 6-methyl-	13151-10-5	3140	1091.23	842	est	137.6 T		implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	(N N')
1-Pentene, 3,3-dimethyl-	3404-73-7	3370	1135.29	657	exp	77.5 E		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
1-Tridecene	2437-56-1	4960	1480.49	1289	exp	232.8 E		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1-Undecene, 5-methyl-	74630-38-9	3690	1198.04	1140	est	205.0 T		implicit	Frack/Geogenic	(Y Y'), (N N')	-	-	-	-	(N N')
1-Undecene, 7-methyl-	74630-42-5	4850	1453.66	1146	est	205.0 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
1,2-Diheptylcyclopropene	35365-53-8	4510	1373.33	1714	est	308.6 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1,2-Dipentylcyclopropene		3500	1160.78	1316	est	235.7 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1,3,5-Cycloheptatriene	544-25-2	950	721.67	785	exp	117.0 E		implicit	Frack/Geogenic	-	-	(Y N')	-	-	(Y N')
1,3,5-Cycloheptatriene, 2,4-diethyl-7,7-dimethyl-		3720	1204.17	1298	est	232.0 T		implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
1,3,5-Cycloheptatriene, 3,7,7-trimethyl-	3479-89-8	4160	1295.83	1010	est	172.8 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1,3,8-p-Menthatriene	21195-59-5	3110	1085.96	1029	est	196.6 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
1,5-Hexadiene, 2,5-dipropyl-		5010	1492.68	1148	est	206.5 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
1,6,9-Tetradecatriene		4370	1342.22	1419	est	256.6 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
1,9-Tetradecadiene		4040	1270.83	1411	est	248.8 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1,E-8,Z-10-Pentadecatriene		5030	1497.56	1518	est	278.3 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
10-Heneicosene (c,t)	95008-11-0	4740	1426.83	2117	est	369.7 T		implicit	Frack/Geogenic	(N N')	(N N')	(N N')	-	-	(N N')
2-Butyl-1-decene	51655-65-3	4040	1270.83	1380	est	249.1 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
2-Dodecene, (E)-	7206-13-5	4330	1333.33	1202	exp	216.2 T		implicit	Frack/Geogenic	-	-	(N N')	-	-	-
2-Hexene, 4-ethyl-2,3-dimethyl-		1930	885.00	913	est	164.9 T		implicit	Frack/Geogenic	-	(Y N')	-	-	(Y N')	-
2-Pentene, 2,4,4-trimethyl-	107-40-4	1970	891.67	727	exp	104.9 E		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
2-Pentene, 3,4,4-trimethyl-	598-96-9	2030	901.67	752	exp	112.0 E		implicit	Frack/Geogenic	-	-	(N N')	-	-	-
2-Tetradecyne	638-60-8	4730	1424.39	1464	exp	252.5 T		implicit	Frack/Geogenic	(Y Y')	-	-	-	-	-
2-Tridecene, (Z)-	41446-59-7	4480	1366.67	1311	exp	235.3 T		implicit	Frack/Geogenic	-	-	-	-	-	(Y N')
2,3,3-Trimethyl-1-hexene	700000-97-1	1650	838.33	825	exp	132.0 T		implicit	Frack/Geogenic	-	(Y Y')	(Y Y')	-	(Y Y')	-
2,4,4-Trimethyl-1-hexene	51174-12-0	2020	900.00	799	est	132.0 T		implicit	Frack/Geogenic	-	-	(N N')	-	-	-
2,4,6-Trimethyl-1-nonene	55771-40-9	7360	2186.21	1053	est	200.1 T		implicit	Frack/Geogenic	-	-	(N N')	-	-	-
3-Dodecene, (E)-	7206-14-6	3380	1137.25	1193	exp	212.2 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
3-Eicosene, (E)-	74685-33-9	4360	1340.00	2017	est	354.3 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	(N N')
3-Ethyl-3-phenyl-1-pentene	19781-34-1	4340	1335.56	1296	est	229.7 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
3-Hexadecene, (Z)-	34303-81-6	5180	1535.90	1620	est	288.1 T		implicit	Frack/Geogenic	(Y Y')	-	-	-	-	-
3-Hexadecyne	61886-62-2	5360	1582.05	1629	est	287.0 T		implicit	Frack/Geogenic	(Y Y')	(N N')	-	-	-	-
3-Octadecene, (E)-	7206-19-1	5160	1530.77	1818	est	322.2 T		implicit	Frack/Geogenic	-	-	-	(N Y')	-	(N N')
3-Octadecyne	61886-64-4	5680	1665.79	1828	est	315.4 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
3-Octyne, 7-methyl-	37050-06-9	4090	1281.25	869	est	145.3 T		implicit	Frack/Geogenic	(N N')	-	-	-	-	-
3-Tetradecene, (E)-	41446-68-8	3830	1227.08	1393	exp	251.6 T		implicit	Frack/Geogenic	(N N'), (Y Y')	(Y N')	-	-	-	(Y Y')
3-Tridecene, (E)-	41446-57-5	3870	1235.42	1289	exp	232.3 T		implicit	Frack/Geogenic	(Y Y')	-	-	-	-	(Y Y')

Compound Name	CAS RN	1D Retention (sec)	1D RI	NIST RI	RI Type	BP (°C)	BP Type	Disclosure	Compound Source	Sample Name A	B	C	D	E	F
Alkenes cont.										Confidence Assignment (RI BP)					
3-Undecene, 7-methyl-, (Z)-		4700	1417.07	1158	est	207.4	T	implicit	Frack/Geogenic	(N N')	-	-	-	-	-
3-Undecene, 9-methyl-, (E)-		3490	1158.82	1158	est	207.4	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	(N N')
3,5-Dodecadiene, 2-methyl-	28980-74-7	3690	1198.04	1265	est	235.6	T	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
4-Nonene, 3-methyl-, (Z)-		3760	1212.50	959	est	163.9	T	implicit	Frack/Geogenic	-	-	-	-	-	(N N')
4-Octene, 2,3,7-trimethyl-, [S-(E)]-		6160	1800.00	930	est	176.5	T	implicit	Frack/Geogenic	(N N')	-	-	-	-	-
4-Tetradecene, (E)-	41446-78-0	4240	1313.33	1388	exp	251.6	T	implicit	Frack/Geogenic	-	(Y Y')	(Y Y')	-	-	-
4-Tetradecene, (Z)-	41446-65-5	4500	1371.11	1389	exp	251.6	T	implicit	Frack/Geogenic	(Y Y')	-	-	-	-	(Y N')
4-Tetradecyne	60212-33-1	4160	1295.83	1427	exp	255.4	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	(Y Y')
4-Tridecene	60186-79-0	4690	1414.63	1284	exp	232.3	T	implicit	Frack/Geogenic	(N N')	-	-	-	-	-
4-Undecene, 10-methyl-, (E)-		4640	1402.44	1158	est	NA		implicit	Frack/Geogenic	-	-	(N -)	-	-	-
5-Eicosene, (E)-	74685-30-6	5060	1505.13	2017	est	354.3	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	(N N')
5-Octadecene, (E)-	7206-21-5	5010	1492.68	1818	est	322.2	T	implicit	Frack/Geogenic	(N N')	-	(N N')	-	-	-
5-Tetradecene, (E)-	41446-66-6	4130	1289.58	1386	exp	251.6	T	implicit	Frack/Geogenic	-	-	-	-	-	(Y N')
5-Tridecene, (E)-	23051-84-5	3560	1172.55	1283	exp	232.3	T	implicit	Frack/Geogenic	(N N'), (Y Y')	(N N')	-	-	-	-
5-Tridecene, (Z)-	25524-42-9	4280	1322.22	1280	exp	232.3	T	implicit	Frack/Geogenic	(Y Y')	-	-	-	-	(N N')
5-Undecene, (Z)-	764-96-5	2840	1038.60	1084	exp	192.3	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
6-Dodecyne	6975-99-1	4290	1324.44	1224	exp	281.2	E	implicit	Frack/Geogenic	(N N')	-	-	-	-	-
6-Tetradecene, (E)-	41446-64-4	3840	1229.17	1383	exp	251.6	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
7-Hexadecene, (Z)-	35507-09-6	4420	1353.33	1620	est	288.1	T	implicit	Frack/Geogenic	(N N')	-	(N N')	-	-	(N N')
7-Octadecyne, 2-methyl-	35354-38-2	9400	3035.00	1863	est	327.8	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
7-Octylidenebicyclo[4.1.0]heptane		4190	1302.22	1522	est	280.7	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
7-Pentadecyne		4500	1371.11	1530	est	272.7	T	implicit	Frack/Geogenic	-	(N N'), (Y Y')	-	-	-	-
7-Tetradecene	10374-74-0	5030	1497.56	1421	est	251.6	T	implicit	Frack/Geogenic	-	-	(Y N')	-	-	-
7-Tetradecene, (Z)-	41446-60-0	3980	1258.33	1374	exp	251.6	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	(Y Y')
7-Tetradecyne	35216-11-6	4340	1335.56	1416	exp	255.4	T	implicit	Frack/Geogenic	(Y Y'), (N N')	(Y Y')	-	-	-	-
8-Heptadecene	54290-12-9	5370	1584.62	1719	est	305.4	T	implicit	Frack/Geogenic	(N N'), (Y Y')	-	-	-	-	-
8-Hexadecyne	19781-86-3	3920	1245.83	1629	est	289.3	T	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	-
9-Eicosyne	71899-38-2	6510	1906.45	2027	est	351.3	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
9-Nonadecene	31035-07-1	4930	1473.17	1880	exp	338.5	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
9-Octadecene, (E)-	7206-25-9	4500	1371.11	1818	est	322.2	T	implicit	Frack/Geogenic	(N N')	-	(Y Y')	-	-	(N N')
9-Octadecyne	35365-59-4	4330	1333.33	1828	est	321.2	T	implicit	Frack/Geogenic	(Y Y')	-	-	-	(Y Y')	(Y Y')
Bicyclo[10.1.0]tridec-1-ene		4350	1337.78	1472	est	268.3	T	implicit	Frack/Geogenic	(Y Y')	(N N')	-	-	-	-
Bicyclo[6.1.0]nonane, 9-(1-methylethylidene)-	56666-90-1	4450	1360.00	1242	est	223.5	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Bicyclo[7.7.0]hexadec-1(9)-ene		5140	1525.64	1860	est	325.8	T	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	-
1-Decene	872-05-10	4823	1477.32	1596	exp	239.9	E	implicit	Frack/Geogenic	-	-	-	-	-	(N N')
1-Decene, 8-methyl-	61142-79-9	4838	1480.85	1602	exp	240.8	T	implicit	Frack/Geogenic	-	-	-	-	-	(N N')
1-Docosene	1599-67-4	4852	1484.37	1608	exp	241.6	E	implicit	Frack/Geogenic	(N N')	(N N'), (Y Y')	(N N')	-	-	(N N')
1-Heptene, 4-methyl-	13151-05-9	4866	1487.89	1615	exp	242.4	E	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1-Heptene, 6-methyl-	5026-76-7	4880	1491.42	1621	exp	243.3	E	implicit	Frack/Geogenic	-	-	(N N')	-	-	-
1-Hexadecene	629-73-3	4894	1494.94	1627	exp	244.1	E	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1-Hexene, 3,3,5-trimethyl-	13427-43-6	4908	1498.46	1634	est	244.9	T	implicit	Frack/Geogenic	-	-	-	-	-	(N N')
1-Hexene, 4,5-dimethyl-	16106-59-6	4922	1501.99	1640	exp	245.8	T	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	-
1-Nonadecene	18435-45-6	4936	1505.51	1646	exp	246.6	E	implicit	Frack/Geogenic	-	(N N')	-	(Y Y')	-	-
1-Nonene, 4,6,8-trimethyl-	54410-98-10	4950	1509.03	1653	est	247.4	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1-Octadecyne	629-89-1	4964	1512.56	1659	est	248.2	E	implicit	Frack/Geogenic	-	-	-	-	-	(Y Y')
1-Octene, 3,7-dimethyl-		4978	1516.08	1665	exp	249.1	T	implicit	Frack/Geogenic	(N N')	-	-	-	-	(N N')
1-Octene, 4-methyl-	13151-12-8	4992	1519.60	1672	est	249.9	T	implicit	Frack/Geogenic	(N N')	-	-	-	-	-
1-Octene, 6-methyl-	13151-10-6	5006	1523.13	1678	est	250.7	T	implicit	Frack/Geogenic	(N N')	(N N')	-	-	-	(N N')
Compound Name	**CAS RN**	**1D Retention (sec)**	**1D RI**	**NIST RI**	**RI Type**	**BP (°C)**	**BP Type**	**Disclosure**	**Compound Source**	**Sample Name A**	**B**	**C**	**D**	**E**	**F**
Aromatics										Confidence Assignment (RI BP)					
1-Methyl-2-n-hexylbenzene	1595-10-4	4180	1300.00	1629	exp	247.5	T	implicit	Frack/Geogenic	-	(N Y')	-	-	-	-
1,1'-Biphenyl, 3-methyl-	643-93-6	5040	1500.00	1477	exp	272.7	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-

Compound Name	CAS RN	1D Retention (sec)	1D RI	NIST RI	RI Type	BP (°C)	BP Type	Disclosure	Compound Source	Sample Name A	B	C	D	E	F
Aromatics Cont.										Confidence Assignment (RI BP)					
1,1'-Biphenyl, 3,4'-dimethyl-	7383-90-6	5050	1502.56	2246	exp	289 E		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
1H-Indene, 1-methyl-3-propyl-		4450	1360.00	1378	est	265.7 T		no	Frack/Geogenic	-	(Y N')	-	-	-	-
1H-Indene, 1,3-dimethyl-	2177-48-2	4780	1436.59	1179	est	228.9 T		no	Frack/Geogenic	-	(N N')	-	-	-	-
1H-Indene, 2,3-dihydro-1,1-dimethyl-	4912-92-9	3320	1125.49	1090	exp	191 E		no	Frack/Geogenic	-	(Y Y')	-	-	-	-
1H-Indene, 2,3-dihydro-1,1,5-trimethyl-	40650-41-7	3430	1147.06	1294	est	217.2 T		no	Frack/Geogenic	-	(N Y'), (Y Y')	-	-	-	-
1H-Indene, 2,3-dihydro-1,1,6-trimethyl-	14276-95-0	3560	1172.55	1294	est	212.8 T		no	Frack/Geogenic	-	(N Y'), (Y Y')	-	-	-	-
1H-Indene, 2,3-dihydro-1,3-dimethyl-	4175-53-5	3040	1073.68	1135	exp	208.7 T		no	Frack/Geogenic	-	(Y N')	-	-	-	-
1H-Indene, 2,3-dihydro-1,6-dimethyl-	17059-48-2	3340	1129.41	1174	exp	213.5 T		no	Frack/Geogenic	-	(Y Y')	-	-	-	-
1H-Indene, 2,3-dihydro-4-propyl-		3960	1254.17	1359	est	234.5 T		no	Frack/Geogenic	-	(N Y')	-	-	-	-
1H-Indene, 2,3-dihydro-4,7-dimethyl-	6682-71-9	3610	1182.35	1251	exp	226.6 T		no	Frack/Geogenic	-	(Y N')	-	-	-	-
1H-Indene, 2,3-dihydro-5-methyl-	874-35-1	3040	1073.68	1124	exp	202 E		no	Frack/Geogenic	-	(Y Y')	-	-	-	-
1H-Indene, 3-ethenyl-2,3-dihydro-1,1-dimethyl-		4580	1388.89	1332	est	231.5 T		no	Frack/Geogenic	-	(Y N')	-	-	-	-
1H-Indene, octahydro-2,2,4,4,7,7-hexamethyl-, trans-	54832-83-6	4250	1315.56	1427	exp	239.4 T		no	Frack/Geogenic	(N Y'), (Y Y')	-	(Y Y')	-	(N Y'), (Y Y')	(N Y'), (Y Y')
2,2'-Dimethylbiphenyl	605-39-0	5470	1610.53	1594	est	259 E		implicit	Frack/Geogenic	-	(Y N'), (N Y')	-	-	-	-
2,4-Dimethylstyrene	2234-20-0	3090	1082.46	1081	exp	206 E		implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
4,4'-Dimethylbiphenyl	613-33-2	5090	1512.82	1589	exp	295 E		implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
4a(2H)-Naphthalenemethanol, octahydro-		5330	1574.36	1417	est	258 T		no	Suspect Frack	(N N')	(N N')	-	-	-	-
9-Methyl-S-octahydrophenanathracene		6000	1754.29	1766	est	314 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Acenaphthylene, 1,2,2a,3,4,5-hexahydro-	480-72-8	4170	1297.92	1360	exp	249 E		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Anthracene, 1,2,3,4,5,6,7,8-octahydro-	1079-71-6	5540	1628.95	1679	exp	305.6 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Anthracene, 1,2,3,4,5,6,7,8-octahydro-1-methyl-		5600	1644.74	1714	est	317.1 T		implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Benzene, (1-cyclohexylethyl)-	4413-16-5	4710	1419.51	1489	est	265 E		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, (1-ethyl-1-methylpropyl)-	1985-97-3	3640	1188.24	1206	est	205 E		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, (1-ethyl-1-propenyl)-	4701-36-4	3520	1164.71	1145	exp	204 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, (1-methylethyl)-	98-82-8	2140	920.00	919	exp	153 E		explicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, (1-methylpropyl)-	135-98-8	2580	993.33	1000	exp	173.5 E		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, (1,1-dimethylpropyl)-	2049-95-8	2910	1050.88	1083	exp	192.4 E		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, (1,3-dimethylbutyl)-	19219-84-2	3430	1147.06	1220	exp	207.7 T		implicit	Frack/Geogenic	-	(Y Y'), (N N')	-	-	-	-
Benzene, (2,4-dimethylcyclopentyl)-		4290	1324.44	1356	est	244.5 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, (cyclohexylmethyl)-	4410-75-7	4310	1328.89	1454	est	255.6 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Benzene, (methoxymethyl)-	538-86-3	2160	923.33	973	exp	170 E		no	Frack/Geogenic	-	(Y N')	-	-	-	-
Benzene, (phenoxymethyl)-	946-80-5	3990	1260.42	1548	exp	286.5 E		no	Suspect Frack	-	(N N')	-	-	-	-
Benzene, 1-(1-formylethyl)-4-(1-buten-3-yl)-		4730	1424.39	1454	est	269.8 T		no	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1-(1-methyl-2-propenyl)-4-(2-methylpropyl)-		4580	1388.89	1365	est	250.3 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1-(1-methylethenyl)-2-(1-methylethyl)-	5557-93-7	3830	1227.08	1261	exp	223 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1-(1-methylethenyl)-3-(1-methylethyl)-	1129-29-9	3560	1172.55	1144	exp	219.9 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1-(1,1-dimethylethyl)-4-ethenyl-	1746-23-2	3750	1210.42	1201	exp	219 E		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1-cyclohexyl-3-methyl-	4575-46-6	4380	1344.44	1467	est	262.6 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Benzene, 1-ethyl-3-(1-methylethyl)-	4920-99-4	3420	1145.10	1094	exp	192.5 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1-ethyl-3-methyl-	620-14-4	2240	936.67	950	exp	161.3 E		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1-ethyl-4-(1-methylethyl)-	4218-48-8	3180	1098.25	1105	exp	197.1 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1-methyl-2-(1-ethylpropyl)-	54410-74-1	3300	1121.57	1192	exp	217.4 T		implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Benzene, 1-methyl-3-(1-methylethyl)-	535-77-3	2950	1057.89	1010	exp	175.1 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1-methyl-3-hexyl-	1595-03-5	3930	1247.92	1404	exp	245.1 T		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Benzene, 1-methyl-4-(1-methylethyl)-	99-87-6	2870	1043.86	1014	exp	177.1 E		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1-methyl-4-(1-methylpropyl)-	1595-16-0	3100	1084.21	1100	exp	195.9 T		implicit	Frack/Geogenic	-	(Y Y'), (N N')	-	-	-	-
Benzene, 1-methyl-4-(2-methylpropyl)-		3130	1089.47	1134	exp	196 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1-methyl-4-(phenylmethyl)-	620-83-7	4720	1421.95	1580	exp	286 E		implicit	Frack/Geogenic	-	(N N')	-	-	-	-
Benzene, 1-pentenyl-	826-18-6	3480	1156.86	1199	est	217 E		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1,2,3-trimethyl-	526-73-8	2390	961.67	1010	exp	176.1 E		explicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Benzene, 1,2,4-triethyl-	877-44-1	3350	1131.37	1224	exp	218 E		implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Benzene, 1,2,4-trimethyl-5-(1-methylethyl)-	10222-95-4	3690	1198.04	1233	exp	221 E		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1,2,4,5-tetramethyl-	95-93-2	2940	1056.14	1107	exp	196.8 E		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1,3-dimethyl-5-(1-methylethyl)-	4706-90-5	2940	1056.14	1103	exp	193.9 T		implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-

Compound Name	CAS RN	1D Retention (sec)	1D RI	NIST RI	RI Type	BP (°C)	BP Type	Disclosure	Compound Source	Sample Name A	B	C	D	E	F
Aromatics Cont.										Confidence Assignment (RI BP)					
Benzene, 1,3,5-trimethyl-2-propyl-		3780	1216.67	1263	exp	232.1	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1,4-diethyl-2-methyl-	13632-94-5	3150	1092.98	1144	exp	206.7	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1,4-dimethyl-2-(1-methylethyl)-	4132-72-3	3530	1166.67	1119	exp	196.2	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 1,4-dimethyl-2-(2-methylpropyl)-	55669-88-0	3600	1180.39	1224	exp	222.5	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, 2-ethyl-1,4-dimethyl-	1758-88-9	2720	1017.54	1067	exp	186.9	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, butyl-	104-51-8	2600	996.67	1047	exp	183.3	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, cyclohexyl-	827-52-1	3930	1247.92	1312	exp	240.1	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Benzene, hexyl-	1077-16-3	3670	1194.12	1247	exp	226.1	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, nonyl-	1081-77-2	5030	1497.56	1555	exp	280.5	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, octyl-	2189-60-8	4610	1395.56	1454	exp	264.5	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, pentamethyl-	700-12-9	3760	1212.50	1654	est	232	E	implicit	Frack/Geogenic	-	(N Y')	-	-	-	-
Benzene, pentyl-	538-68-1	3160	1094.74	1145	exp	205.4	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzene, propyl-	103-65-1	2000	896.67	945	exp	159.2	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Benzeneethanol, ö-methyl-		5440	1602.63	1249	est	NA		no	Suspect Frack	-	(N -)	-	-	-	-
Benzeneethanol, _,ö-dimethyl-		4110	NA	NA		NA		no	Suspect Frack	-	(- -)	-	-	-	-
Benzenemethanol, _-methyl-, (S)-		2560	NA	NA		NA		no	Suspect Frack	-	(- -)	-	-	-	-
Benzenemethanol, _,_-dimethyl-		2690	NA	NA		NA		no	Suspect Frack	(- -)	(- -)	-	-	-	-
Benzoic acid, 2-(benzoylthio)thiazol-4-yl ester		3650	1190.20	2822	est	533	T	no	Suspect Frack	-	-	(N N')	-	-	-
Diphenylmethane	101-81-5	4620	1397.78	1412	exp	265	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Ethylbenzene	100-41-4	1430	801.67	850	est	136.1	E	explicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Indan, 1-methyl-	767-58-8]	2750	1022.81	1078	exp	193.4	T	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene	91-20-3	3230	1107.84	1162	exp	217.9	E	explicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, 1-methyl-7-(1-methylethyl)-	490-65-3	5220	1546.15	1592	est	284.2	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Naphthalene, 1,2,3,4-tetrahydro-	119-64-2	3140	1091.23	1147	exp	207.6	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, 1,2,3,4-tetrahydro-1-methyl-	1559-81-5	3470	1154.90	1207	exp	220.6	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, 1,2,3,4-tetrahydro-1,1-dimethyl-	1985-59-7	3690	1198.04	1263	exp	221.5	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Naphthalene, 1,2,3,4-tetrahydro-1,1,6-trimethyl-	475-03-6	4040	1270.83	1255	exp	240	E	implicit	Frack/Geogenic	-	(Y Y'), (N Y')	-	-	-	-
Naphthalene, 1,2,3,4-tetrahydro-1,4-dimethyl-	4175-54-6	4030	1268.75	1283	exp	234.4	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Naphthalene, 1,2,3,4-tetrahydro-1,8-dimethyl-	25419-33-4	3390	1139.22	1344	exp	241.7	T	implicit	Frack/Geogenic	-	(N N'), (Y N')	-	-	-	-
Naphthalene, 1,2,3,4-tetrahydro-2-methyl-	3877-19-8	3420	1145.10	1207	exp	221	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, 1,2,3,4-tetrahydro-2,2,5,7-tetramethyl-	23342-25-8	4560	1384.44	1445	exp	266.6	T	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, 1,2,3,4-tetrahydro-2,5,8-trimethyl-	30316-17-7	4490	1368.89	1454	est	261.9	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Naphthalene, 1,2,3,4-tetrahydro-5-methyl-	2809-64-5	3790	1218.75	1280	exp	234	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, 1,2,3,4-tetrahydro-5,7-dimethyl-	21693-54-9	4260	1317.78	1374	exp	250	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Naphthalene, 1,2,3,4-tetrahydro-6-propyl-	42775-77-9	4150	1293.75	1353	exp	264.8	T	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, 1,2,3,4-tetramethyl-	3031-15-0	5430	1600.00	1684	est	314	T	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, 1,4,5-trimethyl-	2131-41-1	4810	1443.90	1515	exp	290.3	T	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, 1,6,7-trimethyl-	2245-38-7	4910	1468.29	1545	exp	285	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, 2-(1-methylethyl)-	2027-17-0	4740	1426.83	1435	exp	268	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Naphthalene, 2-butyldecahydro-	6305-52-8	4490	1368.89	1432	exp	263.9	T	implicit	Frack/Geogenic	(Y N')	(Y N')	-	-	-	(Y N')
Naphthalene, 2-ethyl-	939-27-5	4240	1313.33	1382	exp	258	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, 2-ethyl-1,2,3,4-tetrahydro-	32367-54-7	3980	1258.33	1313	exp	235	E	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Naphthalene, 2-ethyldecahydro-	1618-23-1	3550	1170.59	1267	exp	225.4	T	implicit	Frack/Geogenic	(Y N')	(Y N')	-	-	-	-
Naphthalene, 2-methyl-	91-57-6	3780	1216.67	1273	exp	241.1	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, 2,3-dimethyl-	581-40-8	4350	1337.78	1426	exp	268	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, 2,6-dimethyl-	581-42-0	4300	1326.67	1388	exp	262	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, 3-(1,1-dimethylethyl)-1,2-dihydro-	55682-81-0	5030	1497.56	1452	est	262.9	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Naphthalene, 5-ethyl-1,2,3,4-tetrahydro-	42775-75-7	3940	1250.00	1354	exp	245	E	implicit	Frack/Geogenic	-	(N N'), (Y N')	-	-	-	-
Naphthalene, 6-butyl-1,2,3,4-tetrahydro-	30654-45-6	4700	1417.07	1537	exp	282.5	T	implicit	Frack/Geogenic	-	(N N'), (Y N')	-	-	-	-
Naphthalene, 6-ethyl-1,2,3,4-tetrahydro-	22531-20-0	4140	1291.67	1339	exp	244	E	implicit	Frack/Geogenic	-	(Y Y'), (N N')	-	-	-	-
Naphthalene, decahydro-, trans-	493-02-7	2630	1001.75	1058	exp	187.3	E	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, decahydro-1,5-dimethyl-	66552-62-3	3460	1152.94	1223	est	218.3	T	implicit	Frack/Geogenic	-	(Y Y')	-	-	-	-
Naphthalene, decahydro-1,6-dimethyl-	1750-51-2	3330	1127.45	1223	est	218.3	T	implicit	Frack/Geogenic	(Y N')	(Y Y')	-	-	-	-
Naphthalene, decahydro-1,6-dimethyl-4-(1-methylethyl)-	29788-41-8	3530	1166.67	1455	exp	265.1	T	implicit	Frack/Geogenic	-	(N N')	-	-	-	(Y N')

Compound Name	CAS RN	1D Retention (sec)	1D RI	NIST RI	RI Type	BP (°C)	BP Type	Disclosure	Compound Source	Sample Name A	B	C	D	E	F
										Confidence Assignment (RI BP)					
Aromatics Cont.															
Naphthalene, decahydro-2-methyl-	2958-76-1	3040	1073.68	1159	exp	204.6	T	implicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Naphthalene, decahydro-2,2-dimethyl-		5170	NA	NA		213.6	T	implicit	Frack/Geogenic	(- N')	-	-	-	-	-
Naphthalene, decahydro-2,3-dimethyl-		3320	NA	NA		213.6	T	implicit	Frack/Geogenic	-	(- Y')	-	-	-	-
Naphthalene, decahydro-2,6-dimethyl-	1618-22-0	3250	1111.76	1223	est	218.3	T	implicit	Frack/Geogenic	-	(N N'), (Y Y')	-	-	-	-
p-Xylene	106-42-3	3470	1154.90	860	exp	137.5	E	explicit	Frack/Geogenic	-	(N N'), (Y N')	-	-	-	-
Phenol	108-95-2	2140	920.00	957	exp	181.8	E	explicit	Frack/Geogenic	-	(Y N')	-	-	-	-
Toluene	108-88-3	940	720.00	757	exp	111	E	explicit	Frack/Geogenic	(Y Y')	(Y Y')	-	-	(Y Y')	-
Carbonyls															
1-Adamantyl methyl ketone	1660-04-4	3950	NA	NA		262.3	T	no	Suspect Frack	-	(- Y')	-	-	-	-
1-Propanone, 1-phenyl-	93-55-0	3880	1237.5	1146	exp	217.5	E	no	Suspect Frack	-	-	(Y Y')	-	-	-
1,1,3a-Trimethyl-1a,3a,5,6-tetrahydro-1H-cyclopropa[c]pentalen-4-one		4060	NA	NA		243.2	T	no	Suspect Frack	-	(- Y')	-	-	-	-
1,2-Dimethyl-4-trifluoroacetoxycyclohexane		4340	NA	NA		200.0	T	no	Suspect Frack	-	-	-	-	-	(- N')
1,2,3,5,6,7-Hexahydro-inden-4-one		4260	1317.78	1192	est	254.3	T	no	Suspect Frack	-	(N N')	-	-	-	-
1(2H)-Naphthalenone, 3,4-dihydro-	529-34-0	4070	1277.08	1358	exp	115.0	E	no	Suspect Frack	-	(Y N')	-	-	-	-
1H-Inden-1-one, 2,3-dihydro-	83-33-0	3620	1184.31	1218	exp	243.0	E	no	Suspect Frack	-	(Y N')	-	-	-	-
2-Butanol, 3-methyl-, acetate	5343-96-4	3170	1096.49	812	exp	122.4	E	no	Suspect Frack	-	-	-	-	(N N')	-
2-Cyclohexen-1-one, 4-methyl-4-phenyl-	17429-36-6	4910	1468.29	1581	est	254.1	T	no	Suspect Frack	-	(N Y'), (Y N')	-	-	-	-
2-Ethyl-3-methylene-indan-1-one		4620	NA	NA		279.8	T	no	Suspect Frack	-	(- N')	-	-	-	-
2-Nonanone	821-55-6	2770	1026.32	1071	exp	195.0	E	no	Suspect Frack	-	(Y N')	(Y N')	-	-	-
2-Nonanone, 9-hydroxy-		6210	1815.15	1295	est	268.9	T	no	Suspect Frack	-	(N N')	-	-	-	-
2-Propenoic acid, 2-methyl-, ethenyl ester	25719-55-5	5400	NA	NA		111.5	E	no	Suspect Frack	-	-	-	-	-	(- N')
2-Propylhept-3-enoic acid, phenylthio ester		3690	1198.04	2019	est	359.0	T	no	Suspect Frack	-	(N N')	-	-	-	-
2,3,4-Trimethyl-hex-3-enal		3430	1147.06	1002	est	191.6	T	implicit	Frack/Geogenic	(N N')	-	-	-	-	-
2,4-Decadienal	2363-88-4	3880	1237.50	1285	exp	277.7	E	implicit	Subsurf. Rxn.	-	(Y N')	-	-	-	-
2(3H)-Furanone, 5-butyldihydro-	104-50-7	3500	1160.78	1216	exp	234.0	E	no	Suspect Frack	-	(Y N')	-	-	-	-
2(3H)-Furanone, 5-ethyldihydro-	695-06-7	2390	961.67	1007	exp	215.5	E	no	Suspect Frack	-	(Y N')	(Y N')	-	-	-
2(3H)-Furanone, 5-heptyldihydro-	104-67-6	6090	1780.00	1531	exp	286.0	E	no	Suspect Frack	-	(N N')	-	-	-	-
2(3H)-Furanone, 5-hexyldihydro-	706-14-9	4470	1364.44	1428	exp	304.4	E	no	Suspect Frack	(Y N')	(Y N'), (N N')	-	-	-	-
2(3H)-Furanone, dihydro-5-methyl-	108-29-2	1780	860.00	917	exp	207.5	E	no	Suspect Frack	(Y N')	(Y N')	-	-	-	-
2(3H)-Furanone, dihydro-5-pentyl-	104-61-0	4010	1264.58	1324	exp	266.6	T	no	Suspect Frack	-	(Y Y')	-	-	-	-
2(3H)-Furanone, dihydro-5-propyl-	105-21-5	2950	1057.89	1108	exp	226.3	T	no	Suspect Frack	-	(Y N')	-	-	-	-
2(5H)-Furanone, 5-methyl-	591-11-7	1680	843.33	916	exp	210.0	T	no	Suspect Frack	(Y N')	-	-	-	-	-
2H-Benzocyclohepten-2-one, 3,4,4a,5,6,7,8,9-octahydro-4a-methyl-, (S)-		4400	1348.89	1477	est	287.9	T	no	Suspect Frack	-	(N N')	-	-	-	-
2H-Pyran-2-one, 6-heptyltetrahydro-	713-95-1	6860	2019.35	1675	exp	126.0	E	no	Suspect Frack	-	(N N')	-	-	-	-
2H-Pyran-2-one, tetrahydro-	542-28-9	2330	951.67	991	exp	219.0	E	no	Suspect Frack	(Y N')	(Y N')	-	-	-	-
2H-Pyran-2-one, tetrahydro-6-methyl-	823-22-3	2600	996.67	1049	exp	231.0	E	no	Suspect Frack	-	-	-	-	(Y N')	-
2H-Pyran-2-one, tetrahydro-6-pentyl-	705-86-2	4590	1391.11	1452	exp	267.2	T	no	Suspect Frack	-	(Y N')	-	-	-	-
2H-Pyran-2-one, tetrahydro-6-propyl-	698-76-0	3630	1186.27	1250	exp	238.0	E	no	Suspect Frack	-	(Y N')	-	-	-	-
3-Heptanone	106-35-4	1550	821.67	866	exp	147.0	E	no	Suspect Frack	-	-	(Y N')	-	-	-
3-Hexen-1-ol, propanoate, (Z)-	33467-74-2	1770	858.33	1079	exp	210.9	T	no	Suspect Frack	-	-	(N N')	-	-	-
3-Hydroxy-3-methyl-2-butanone	115-22-0	1500	813.33	779	exp	140.5	E	no	Suspect Frack	-	-	-	-	(Y N')	-
3-Methylheptyl acetate	72218-58-7	3110	1085.96	1118	est	195.7	T	no	Suspect Frack	-	-	(Y Y')	-	-	-
3,4-Hexanedione, 2,2,5-trimethyl-	20633-03-8	8250	2525.00	1039	est	177.8	T	no	Suspect Frack	-	-	-	-	-	(N N')
3,6-Heptanedione	1703-51-1	2810	1033.33	989	est	208.3	T	no	Suspect Frack	-	(Y N')	-	-	-	-
4-Penten-2-one	13891-87-7	2150	921.67	644	est	93.9	T	no	Suspect Frack	-	-	(N N')	-	(N N')	-
Acetic acid, trifluoro-, 3,7-dimethyloctyl ester		3980	1258.33	1087	est	233.7	T	no	Suspect Frack	(N N')	-	-	-	-	(N Y')
Acetic acid, trifluoro-, tetradecyl ester		9060	2872.73	1617	exp	248.8	T	no	Suspect Frack	-	(N N')	-	-	-	-
Acetophenone	98-86-2	2550	988.33	1042	exp	202.0	E	explicit	Frack	-	(Y N')	-	-	-	-
Acetyl valeryl	96-04-8	3480	1156.86	816	exp	183.9	E	no	Suspect Frack	(N N')	-	-	-	-	-
Benzaldehyde	100-52-7	1920	883.33	933	exp	178.0	E	no	Suspect Frack	(Y Y')	-	-	-	(Y Y')	-
Benzeneacetaldehyde, _-methyl-	93-53-8	2660	1007.02	1082	exp	203.5	E	no	Suspect Frack	-	(Y N')	-	-	-	-
Benzeneacetaldehyde, _,2,5-trimethyl-		3510	1162.75	1343	est	NA		no	Suspect Frack	-	(N -)	-	-	-	-
Butanal, 3,3-dimethyl-2-oxo-, hemihydrate	4480-47-1_	4490	1368.89	858	est	128.2	T	no	Suspect Frack	(N N')	-	-	-	-	-

Compound Name	CAS RN	1D Retention (sec)	1D RI	NIST RI	RI Type	BP (°C)	BP Type	Disclosure	Compound Source	Sample Name A	B	C	D	E	F
Carbonyls Cont.												Confidence Assignment (RI BP)			
Cyclohexanone	108-94-1	1510	815.00	871	exp	155.4	E	explicit	Frack	-	-	(Y N')	-	-	-
Cyclohexanone, 2-cyclohexylidene-	1011-12-7	4030	1268.75	1551	est	295.0	E	no	Suspect Frack	-	(N N')	-	-	-	-
Cyclohexanone, 4-(1,1-dimethylethyl)-	98-53-3	2930	1054.39	1208	exp	114.0	E	no	Suspect Frack	-	-	(N N')	-	-	-
Decanal	112-31-2	4330	1333.33	1185	exp	208.0	E	implicit	Subsurf. Rxn.	(N N'), (Y N')	-	-	-	-	-
Decanoic acid, octyl ester	2306-92-5	8150	2484.00	1978	est	334.7	T	no	Suspect Frack	-	(N N')	-	-	-	-
Ethanedione, diphenyl-	134-81-6	3650	1190.20	1766	exp	347.0	E	no	Suspect Frack	-	-	-	-	-	(N N')
Ethanone, 2,2-dihydroxy-1-phenyl-	1075-06-5	3650	1190.20	1418	est	212.8	E	no	Suspect Frack	(N Y')	(N Y')	-	-	-	-
Hexanal	66-25-1	1050	738.33	776	exp	131.0	E	implicit	Subsurf. Rxn.	-	(Y N')	-	-	-	-
Hexanal, 2-ethyl-	123-05-7	1970	891.67	934	exp	163.0	E	implicit	Subsurf. Rxn.	-	-	(Y N')	-	-	-
Hexanal, 3-(hydroxymethyl)-4-methyl-		4820	1446.34	1119	est	230.7	T	implicit	Subsurf. Rxn.	-	(N N')	-	-	-	-
m-Toluic acid, 4-cyanophenyl ester	13632-94-5	3450	1150.98	2025	est	412.9	T	no	Suspect Frack	-	(N N')	-	-	-	-
Methyl tetradecanoate	124-10-7	6290	1839.39	1708	exp	295.0	E	no	Suspect Frack	-	(Y Y')	-	-	-	-
n-Dodecyl acetate	112-66-3	8620	2679.17	1594	exp	265.0	E	no	Suspect Frack	-	(N N')	-	-	-	-
Octanoic acid, methyl ester	124-07-2	2970	NA	NA		239.0	E	no	Suspect Frack	-	(- N')	-	-	-	-
Oxalic acid, allyl dodecyl ester		6860	2019.35	2036	est	370.6	T	no	Suspect Frack	-	-	-	(Y N')	-	-
Oxalic acid, allyl hexadecyl ester		5590	1642.11	2433	est	428.4	T	no	Suspect Frack	(N N'), (Y N')	(Y N'), (N Y')	(N N')	-	-	(N N')
Oxalic acid, allyl octadecyl ester		5240	1551.28	2632	est	455.5	T	no	Suspect Frack	(N N'), (Y N')	(N N')	(N N')	-	-	(N N')
Oxalic acid, allyl pentadecyl ester		5190	1538.46	2334	est	414.4	T	no	Suspect Frack	(N N'), (Y N')	(N Y')	(N N')	-	-	-
Oxalic acid, allyl tridecyl ester		4590	1391.11	2135	est	385.5	T	no	Suspect Frack	(N N')	-	(N N')	-	-	(N N')
Oxalic acid, butyl cyclohexylmethyl ester		4190	1302.22	1712	est	317.3	T	no	Suspect Frack	(N N')	(Y N'), (N N')	(N N')	-	-	-
Oxalic acid, butyl propyl ester		2900	1049.12	1250	est	231.9	T	no	Suspect Frack	-	-	(N N')	-	-	-
Oxalic acid, cyclobutyl octadecyl ester		7420	2207.41	2764	est	472.4	T	no	Suspect Frack	(Y N')	(N N')	-	-	-	-
Oxalic acid, di(cyclohexylmethyl) ester		3870	1235.42	2073	est	377.4	T	no	Suspect Frack	-	(N N')	-	-	-	(N N')
Oxalic acid, isobutyl nonyl ester		4590	1391.11	1982	est	333.4	T	no	Suspect Frack	-	-	-	(N N')	-	-
Pentanal, 2,2-dimethyl-	14250-88-5	1820	866.67	821	est	136.4	T	implicit	Subsurf. Rxn.	-	-	(Y N')	-	-	-
Pentanoic acid, 10-undecenyl ester	109-52-4	4330	1333.33	1769	est	314.0	T	no	Suspect Frack	(N N')	-	-	-	-	(N N')
Pentyl glycolate	5426-43-7	4640	1402.44	1127	est	197.4	T	no	Suspect Frack	(N N')	-	-	-	-	-
Propanoic acid, 2-methyl-, 2-methylbutyl ester	2445-69-4	3750	1210.42	1002	exp	165.2	T	no	Suspect Frack	-	-	-	-	-	(N N')
Propanoic acid, 2-methyl-, 3-hydroxy-2,4,4-trimethylpentyl ester	74367-34-3	4180	1300.00	1365	exp	249.0	T	no	Suspect Frack	(Y Y')	-	-	-	-	-
Spiro[2.3]hexan-5-one, 4,4-diethyl-		3070	1078.95	1139	est	209.8	T	no	Suspect Frack	-	(Y N')	-	-	-	-
Spiro[3.6]deca-5,7-dien-1-one,5,9,9-trimethyl		4410	1351.11	1473	est	283.5	T	no	Suspect Frack	-	(N N')	-	-	-	-
Tetrahydrofurfuryl acrylate	100666-89-5	2810	1033.33	1105	est	238.6	E	no	Suspect Frack	-	-	(Y N')	-	-	-
Valeric acid, 4-tridecyl ester		6770	1990.32	1914	est	326.5	T	no	Suspect Frack	-	(Y N')	-	-	-	-
Vinyl butyrate	123-20-6	1470	808.33	750	exp	116.0	E	no	Suspect Frack	-	-	(Y Y')	-	(Y N')	-
Vinyl caprylate	818-44-0	9410	3040.00	1173	est	212.0	T	no	Suspect Frack	-	(N N')	-	-	-	-
Z,E-7,11-Hexadecadien-1-yl acetate	53042-79-8	4350	1337.78	1994	est	365.7	T	no	Suspect Frack	-	(N N')	-	-	-	-
(R)-(-)-4-Methylhexanoic acid		2640	NA	NA		215.3	T	no	Subsurf. Rxn.	-	(- Y')	-	-	-	-
2-Octenoic acid	1871-67-6	3500	1160.78	1181	est	260.2	T	no	Suspect Frack	-	(Y N')	-	-	-	-
2-Oxo-n-valeric acid	1821-02-9	3850	1231.25	1011	est	179.0	E	no	Suspect Frack	-	-	(N N')	-	-	-
2-Pentenoic acid	626-98-2	2010	898.33	883	est	204.7	T	no	Subsurf. Rxn.	(Y Y')	-	-	-	-	-
Benzoic acid	65-85-0	3340	1129.41	1161	exp	249.0	E	no	Suspect Frack	(Y N')	(Y Y')	-	-	-	-
Butanoic acid	107-92-6	1020	733.33	807	exp	164.0	E	no	Subsurf. Rxn.	(Y Y')	(Y Y')	-	-	(Y Y')	-
Butanoic acid, 2-methyl-	116-53-0	1520	816.67	839	exp	175.5	E	no	Subsurf. Rxn.	(Y Y')	(Y Y')	-	-	(Y Y')	-
Butanoic acid, 3-methyl-	503-74-2	1460	806.67	830	exp	176.0	E	no	Subsurf. Rxn.	(N Y')	(Y Y')	-	-	(Y Y')	-
Dodecanoic acid	143-07-7	4990	1487.80	1556	exp	298.9	E	no	Subsurf. Rxn.	-	(Y Y')	-	-	-	-
Heptanoic acid	111-14-8	2720	1017.54	1078	exp	222.5	E	no	Subsurf. Rxn.	(Y Y')	(Y Y')	-	-	(Y Y')	-
Hexadecenoic acid, Z-11-	2416-20-8	6950	2048.39	1976	est	368.9	T	no	Subsurf. Rxn.	-	(Y Y')	-	-	-	-
Hexanoic acid	142-62-1	2400	963.33	982	exp	202.5	E	no	Subsurf. Rxn.	-	(Y Y')	-	-	(Y Y')	-
Hexanoic acid, 2-ethyl-	149-57-5	3000	1066.67	1117	exp	227.5	E	no	Subsurf. Rxn.	-	(Y Y')	-	-	-	-
n-Decanoic acid	334-48-5	4150	1293.75	1362	exp	268.7	E	no	Subsurf. Rxn.	(Y Y')	(Y Y')	-	-	(Y Y')	-
n-Hexadecanoic acid	57-10-3	6390	1869.70	1954	exp	390.0	E	no	Subsurf. Rxn.	(Y N')	(Y N'), (N N')	-	-	-	-
Nonanoic acid	112-05-0	3750	1210.42	1272	exp	254.0	E	no	Subsurf. Rxn.	-	(Y Y')	-	-	-	-
Octanoic Acid	124-07-2	3220	1105.88	1173	exp	237.0	E	no	Subsurf. Rxn.	(Y Y')	(Y Y')	-	-	(Y Y')	-
Oleic Acid	112-80-1	9010	2850.00	2134	exp	390.0	E	explicit	Frack/Geogenic	-	(N N')	-	-	-	-

Compound Name	CAS RN	1D Retention (sec)	1D RI	NIST RI	RI Type	BP (°C)	BP Type	Disclosure	Compound Source	Sample Name A	B	C	D	E	F
										Confidence Assignment (RI BP)					
Carbonyls Cont.															
Pentanoic acid	109-52-4	1590	828.33	901	exp	185.0	E	no	Subsurf. Rxn.	(Y Y')	(Y Y')	-	-	(Y Y')	-
Propanoic acid, 2-hydroxy-2-methyl-	594-61-6	1480	810.00	867	est	264.0	E	no	Subsurf. Rxn.	-	-	(Y N'), (N N')	-	-	(Y N')
Propanoic acid, 2-methyl-	79-31-2	940	720.00	732	exp	153.5	T	no	Subsurf. Rxn.	-	(Y Y')	-	-	-	-
Tetradecanoic acid	544-63-8	5720	1676.32	1752	exp	326.0	E	no	Subsurf. Rxn.	-	(Y Y')	-	-	-	-
Undecanoic acid	112-37-8	5360	1582.05	1472	exp	280.0	E	no	Subsurf. Rxn.	(Y N')	(N N')	-	-	-	-
Ethers & Epoxides															
1,2,4,5-Tetroxane, 3,3,6,6-tetramethyl-	1073-91-2	2700	1014.04	945	est	100.8	T	no	Suspect Frack	-	-	(Y N'), (N N')	-	-	-
1,3-Dioxolane, 2-ethyl-4-methyl-	4359-46-0	1230	768.33	799	est	117	E	no	Suspect Frack	-	-	-	-	(Y Y')	-
2,7-Ethanonaphth[2,3-b]oxirene, 1a,2,7,7a-tetrahydro-, (1a_,2ö,7ö,7a_)-		4970	NA	NA		NA		no	Suspect Frack	-	(- -)	-	-	-	-
7-Methylene-9-oxabicyclo[6.1.0]non-2-ene	264628-23-1	4250	1315.56	1019	est	201.1	T	no	Suspect Frack	(N N')	-	-	-	-	-
7-Oxabicyclo[4.1.0]heptane	286-20-4	1370	791.67	731	est	129.5	E	no	Suspect Frack	-	-	(Y Y')	-	-	-
Oxirane, 2-methyl-2-(1-methylpropyl)-	42328-43-8	2510	981.67	717	est	110.8	T	no	Suspect Frack	-	-	-	-	(N N')	-
Oxirane, tetradecyl-	7320-37-8	10210	3455.56	1702	est	323.5	T	no	Suspect Frack	-	(N N')	-	-	-	-
Santolina epoxide		4470	1364.44	991	est	183.9	T	no	Suspect Frack	-	(N N')	-	-	-	-
Halogenated															
1-Iodo-2-methylundecane	73105-67-6	5440	1602.63	1564	est	297	T	no	Subsurf. Rxn.	(N Y')	-	-	-	-	(Y Y'), (N N')
1,1-Dimethyl-3-chloropropanol	1985-88-2	1090	745.00	835	est	178.6	T	no	Subsurf. Rxn.	-	-	-	-	(Y N')	-
1,3-Dioxolane, 2-(3-bromo-5,5,5-trichloro-2,2-dimethylpentyl)-		9250	2961.90	1770	est	341.9	T	no	Subsurf. Rxn.	-	-	(N N')	-	-	-
2-(Chloromethyl)tetrahydropyran	18420-41-2	2960	1059.65	995	est	181.6	E	no	Subsurf. Rxn.	(Y Y')	-	-	-	-	-
2-Chlorocyclohexanol	1561-86-0	2320	950.00	1074	est	218.3	T	no	Subsurf. Rxn.	-	-	(N N')	-	-	-
2-Piperidinone, N-[4-bromo-n-butyl]-		8090	2460.00	1635	est	341.1	T	no	Subsurf. Rxn.	-	(N N')	-	-	-	-
4-Bromoheptane	998-93-6	2670	1008.77	949	est	178.6	E	no	Subsurf. Rxn.	-	-	(Y Y')	-	-	-
5-Iodopentan-2-one		2140	920.00	1069	est	207.6	T	no	Subsurf. Rxn.	-	-	(N N')	-	(N N')	-
Butane, 1-chloro-3,3-dimethyl-		3680	1196.08	758	est	117	E	no	Subsurf. Rxn.	(N N')	-	-	-	-	-
Butane, 2-iodo-3-methyl-	18295-27-7	5110	1517.95	868	exp	136.9	T	no	Subsurf. Rxn.	-	-	(N N')	-	-	-
Chloromethyl hexanoate	66542-51-6	2790	1029.82	1071	exp	178.8	T	no	Suspect Frack	-	(Y Y')	-	-	(Y Y')	-
Chloromethyl octanoate	61413-70-5	3810	1222.92	1278	exp	221.3	T	no	Suspect Frack	-	(Y Y')	-	-	-	-
Chloromethyl pentanoate	77877-94-2	2210	931.67	981	exp	155.9	T	no	Suspect Frack	(Y Y')	(Y Y')	-	-	-	-
Chloromethyl propanoate	5402-53-9	1080	743.33	811	exp	105.7	T	no	Suspect Frack	-	(Y Y')	-	-	(Y Y')	-
Cyclodecene, 3-bromo-	56325-56-5	3310	1123.53	1439	est	241.5	T	no	Subsurf. Rxn.	(N N'), (Y N')	(N N'), (Y N')	-	-	-	-
Cyclohexane, 1-bromo-2-methyl-	6294-39-9	4200	1304.44	1038	est	174.6	T	no	Subsurf. Rxn.	-	(N N')	-	-	-	-
Cyclopropane, 3-chloro-1,1,2,2-tetramethyl-		1970	891.67	795	est	122.6	T	no	Subsurf. Rxn.	-	-	-	-	(Y N')	-
Decane, 4,5-dibromo-, (R*,R*)-		4010	1264.58	1479	est	281.9	T	no	Subsurf. Rxn.	(N N')	-	-	-	-	-
Hexane, 2-bromo-	3377-86-4	2080	910.00	850	est	144	E	no	Subsurf. Rxn.	-	-	(Y Y')	-	-	-
Methane, bromodichloro-	75-27-4	1130	751.67	693	exp	88	E	no	Subsurf. Rxn.	-	-	(Y N')	-	-	-
Methylene Chloride	75-09-2	930	718.33	518	exp	39	E	explicit	Frack	(N N')	-	(N N')	-	-	-
Nonane, 1-iodo-	4282-42-2	10270	3488.89	1327	exp	269	T	no	Subsurf. Rxn.	-	-	-	-	-	(N N')
Pentadec-7-ene, 7-bromomethyl-		4950	1478.05	1893	est	342	T	no	Subsurf. Rxn.	(N N')	-	-	-	-	-
Pentane, 1-chloro-5-iodo-	60274-60-4	2230	935.00	1158	est	227.6	T	no	Subsurf. Rxn.	-	-	-	-	(Y Y')	-
Propanoic acid, 3-iodo-	141-76-4	1650	838.33	1090	est	259.7	T	no	Subsurf. Rxn.	-	-	-	-	(N N')	-
Tetradecane, 1-iodo-	19218-94-1	5660	1660.53	1827	est	329.7	T	no	Subsurf. Rxn.	(N N')	-	(N N')	-	-	(Y N')
Tricyclo[3.3.1.1(3,7)]decane, 2-bromo-	7314-85-4	2880	1045.61	1433	exp	248.6	T	no	Subsurf. Rxn.	-	(N N')	-	-	-	-
Heterocycles															
1,3-Benzodioxol-2-one, hexahydro-, trans-		1250	771.67	1196	est	298.8	T	no	Suspect Frack	-	-	(N N')	-	-	-
1,4-Methano-1H-cyclohepta[d]pyridazine, 4,4a,5,6,7,8,9,9a-octahydro-10,10-dimethyl-		3600	NA	NA		252.7	T	no	Suspect Frack	-	(- N')	-	-	-	-
1,4-Methanophthalazine, 1,4,4a,5,6,7,8,8a-octahydro-1,4,9,9-tetramethyl-,		3490	NA	NA		NA		no	Suspect Frack	-	(- -)	-	-	-	-
1,4-Methanophthalazine, 1,4,4a,5,6,7,8,8a-octahydro-9,9-dimethyl-,		4150	NA	NA		NA		no	Suspect Frack	-	(- -)	-	-	-	-
1(3H)-Isobenzofuranone	87-41-2	3890	1239.58	1272	est	290	E	no	Suspect Frack	-	(Y N')	-	-	-	-
1H-Tetrazole	288-94-8	2600	NA	NA		220.2	T	no	Suspect Frack	(- N')	-	-	-	-	-
2-Azetidinone, 3,3-dimethyl-	4879-95-2	2670	1008.77	778	est	212.1	T	no	Suspect Frack	-	(N N')	-	-	-	-
2-Furanol, tetrahydro-2-methyl-	7326-46-7	1610	831.67	911	exp	155.1	T	no	Suspect Frack	-	-	-	-	(Y N')	-

Compound Name	CAS RN	1D Retention (sec)	1D RI	NIST RI	RI Type	BP (°C)	BP Type	Disclosure	Compound Source	Sample Name A	B	C	D	E	F
										Confidence Assignment (RI BP)					
Heterocycles Cont.															
Aziridine, 1-vinyl-	5628-99-9	2190	928.33	562	est	71.1	T	no	Suspect Frack	-	-	(N N')	-	-	-
Benzothiazole	95-16-9	3380	1137.25	1187	exp	231	E	no	Suspect Frack	-	(Y Y')	-	-	-	-
Carbamic acid, N-(3-oxo-4-isoxazolidinyl)-, benzyl ester		5330	1574.36	1951	est	415.4	T	no	Suspect Frack	-	-	-	-	-	(N N')
Di(1,2,5-oxadiazolo)[3,4-b;3,4-E]pyrazine, 4,8-diacetyl-		1100	NA	NA		714.8	T	no	Suspect Frack	-	-	(- N')	-	-	-
Furan, 2-pentyl-	3777-69-3	2240	936.67	979	exp	167	E	no	Suspect Frack	-	(Y Y')	-	-	-	-
Furan, tetrahydro-2,2-dimethyl-5-(1-methylethyl)-		1860	873.33	919	est	148	T	no	Suspect Frack	-	-	(Y Y')	-	-	-
Oxetane, 3-(1-methylethyl)-	10317-17-6	1090	745.00	664	est	99.6	T	no	Suspect Frack	(Y Y')	-	-	-	-	-
Other															
1-Hexyl-1-nitrocyclohexane		9040	2863.64	1633	est	297.4	T	no	Suspect Frack	(N N')	-	-	-	-	-
1-Hexyl-2-nitrocyclohexane		4580	1388.89	1621	est	297.4	T	no	Suspect Frack	(N N')	(N N')	-	-	-	(N N')
1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	84-69-5	6000	1754.29	1850	exp	327	E	no	Suspect Frack	-	(Y N')	(Y N')	(Y N')	-	-
1,2-Benzenedicarboxylic acid, butyl 2-methylpropyl ester	17851-53-5	6310	1845.45	1972	est	315.7	T	no	Suspect Frack	-	-	-	(N Y')	-	-
1,2-Benzenedicarboxylic acid, diisooctyl ester	27554-26-3	8010	2428.00	2525	exp	384.9	T	no	Suspect Frack	-	(Y Y')	(Y Y')	-	-	-
2-Methylbutanoic anhydride	1468-39-9	3570	1174.51	1190	est	215	E	no	Suspect Frack	(Y Y')	-	-	-	-	-
2,2-Dimethylpropanoic anhydride	1538-75-6	2770	1026.32	1150	est	193	E	no	Suspect Frack	(N N')	-	-	-	(N N')	-
3-Oxo-4-phenylbutyronitrile	19212-27-2	3620	1184.31	1473	est	267.8	T	no	Suspect Frack	-	(N N')	-	-	-	-
4-Benzyloxybenzonitrile	52805-36-4	5280	1561.54	1820	est	532.4	E	no	Suspect Frack	-	-	-	-	-	(N N')
Aromadendran ('2')		4840	1451.22	1114	est	256.5	T	no	suspect frack	-	(N Y')	-	-	-	-
Bicyclo[3.3.1]nonan-9-one, 1,2,4-trimethyl-3-nitro-, (2-endo,3-exo,4-exo)-(.+-.)-		4280	1322.22	1692	est	330.5	T	no	Suspect Frack	(N N')	(N N')	-	-	-	(N N')
Cyclobutane-1,1-dicarboxamide, N,N'-di-benzoyloxy-	33582-68-2	3320	1125.49	3294	est	NA		no	Suspect Frack	-	(N -)	-	-	-	-
Cyclobutylamine	2516-34-9	1340	786.67	684	est	82	E	implicit	Frack	-	-	-	-	(N N')	-
Cyclotetrasiloxane, octamethyl-	556-67-2	9210	2942.86	1011	exp	175	E	explicit	Frack	(N N')	-	(N N'), (Y Y')	-	-	-
Cyclotrisiloxane, hexamethyl-	541-05-9	1310	781.67	1217	est	134	E	no	Suspect Frack	(N N')	-	(N N')	-	-	-
Dibutyl phthalate	84-74-2	6310	1845.45	1924	exp	339.5	E	no	Suspect Frack	(Y N')	-	(Y N')	-	-	-
Ethanethioic acid, S-(2-methylbutyl) ester	69078-80-4	1630	835.00	1040	est	180.8	T	no	Suspect Frack	-	-	(N N')	-	-	-
Hexane, 2-nitro-	14255-44-8	3710	1202.08	935	est	174.1	T	no	Suspect Frack	(N N')	-	-	-	-	-
N,N,O-Triacetylhydroxylamine		3030	1071.93	1122	est	211.1	T	implicit	Frack	-	-	(Y N')	-	-	-
Pentanoyl chloride	638-29-9	1070	741.67	830	est	109	E	no	Suspect Frack	(Y Y')	-	-	-	-	-
Propanenitrile, 2,2'-azobis[2-methyl-	78-67-1	2200	930.00	1308	est	236.3	T	no	Suspect Frack	-	(Y Y')	-	-	-	-
Propanoic acid, 2-methyl-, anhydride	97-72-3	4620	1397.78	992	est	183	E	no	Suspect Frack	(N N')	-	-	-	-	-
Silane, tetramethyl-	75-76-3	9310	2990.48	433	exp	26.5	E	no	Suspect Frack	(N N')	-	(N N')	-	-	-
Tetramethylbutanedinitrile	3333-52-6	2200	930.00	1138	est	264.2	T	no	Subsurf. Rxn.	-	-	-	-	(Y Y')	-
Trimethylaluminum	75-24-1	2510	NA	NA		NA		no	Suspect Frack	(- -)	-	-	-	-	-
Valeric anhydride	2082-59-9	4380	1344.44	1319	est	227	E	no	Suspect Frack	(Y N'), (N Y')	-	-	-	-	-
Suflurous Acids															
Sulfurous acid, 2-ethylhexyl hexyl ester		7310	2168.97	1972	est	340.3	T	no	Suspect Frack	(N N')	-	-	-	-	-
Sulfurous acid, 2-ethylhexyl isobutyl ester		5100	1515.38	1709	est	335.9	T	no	Suspect Frack	-	-	(N N')	-	-	-
Sulfurous acid, 2-ethylhexyl isohexyl ester		5800	1697.37	1908	est	335.9	T	no	Suspect Frack	(N N')	-	(Y N'), (N N')	-	-	(N N')
Sulfurous acid, butyl undecyl ester		8090	2460.00	2135	est	360.5	T	no	Suspect Frack	(N N')	-	-	-	-	-
Sulfurous acid, dodecyl pentyl ester		4610	1395.56	2334	est	390.6	T	no	Suspect Frack	-	(N N')	-	-	-	(N N')
Sulfurous acid, hexadecyl pentyl ester		10200	3450.00	2732	est	446.8	T	no	Suspect Frack	-	(N N')	-	-	-	-
Sulfurous acid, isobutyl pentyl ester		10440	3583.33	1475	est	253.9	T	no	Suspect Frack	-	-	-	-	-	(N N')
Sulfurous acid, octyl 2-propyl ester		4160	1295.83	1674	est	290.2	T	no	Suspect Frack	-	-	(N N')	-	-	-
Sulfurous acid, pentyl tridecyl ester		5020	1495.12	2434	est	405.1	T	no	Suspect Frack	(N N')	-	-	-	-	-