Supplementary Information

Temperature-Dependent Density and Viscosity Prediction of Hydrocarbons: Machine Learning and Molecular Dynamics Simulations

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Details of Hydrocarbons

Due to the large data set, we used the holdout cross-validation technique. Data were divided randomly into three partitions to develop and assess the models: training, validation, and test data sets. First, 70% of 305 molecules (215 molecules) were used to train the models, and second, 15% of 305 molecules (that is, 45 molecules) were used to validate the models during model development. Third, the remaining 15% of 305 molecules (that is, 45 molecules) that do not belong to the training and validation data sets were selected to assess the accuracy of the estimations with the developed models. Therefore, 70%, 15%, and 15% of 305 molecules were used to train, validate, and test models. All these molecules are listed in Table S1 with partition IDs 1, 2, and 3 to indicate if that molecule falls in training, validation, and test data sets.

Table S1: Descriptions of hydrocarbon molecules.

PSU#	Name	Formula	Smiles Code	Partition
1	11-n-butyldocosane	$C_{26}H_{54}$	CCCCCCCCCC[C@H](CCCCCCCCCC)CCCC	1
2	9-n-butyldocosane	$C_{26}H_{54}$	CCCCCCCC[C@@H](CCCCCCCCCCCCC)CCCC	1
3	7-n-butyldocosane	$C_{26}H_{54}$	CCCCCC[C@@H](CCCCCCCCCCCCCCC)CCCC	1
4	5-n-butyldocosane	$C_{26}H_{54}$	CCCCC(CCCCCCCCCCCCCCCCC)CCCC	3
5	7-n-hexyldocosane	$C_{28}H_{58}$	CCCCCCC(CCCCCCCCCCCCCCC)CCCCCC	2
6	9-n-octyldocosane	$C_{30}H_{62}$	CCCCCCCCC(CCCCCCCCCCCCC)CCCCCCCC	3
7	11-n-decyldocosane	$C_{32}H_{66}$	CCCCCCCCCCC(CCCCCCCCCCC)CCCCCCCCCC	1
8	11-n-decylheneicosane	$C_{31}H_{64}$	CCCCCCCCCCC(CCCCCCCCCC)CCCCCCCCCC	1
9	11-Phenyl-heneicosane	$C_{27}H_{48}$	c1cccc(c1)C(CCCCCCCCCC)CCCCCCCCCC	1
10	9-p-Tolyloctadecane	$C_{25}H_{44}$	c1(ccc(cc1)[C@@H](CCCCCCCC)CCCCCCCCC)C	3
11	1,1-Dicyclohexyltertradecane	$C_{26}H_{50}$	C1CCC(CC1)C(CCCCCCCCCCCC)C1CCCCC1	3
12	1,1-Diphenlytetradecane	$C_{26}H_{38}$	c1ccc(cc1)C(c1ccccc1)CCCCCCCCCCCC	1
13	1,1-Diphenyll-tetradecene	$C_{26}H_{36}$	c1ccc(cc1)C(=CCCCCCCCCCCC)c1ccccc1	2
15	1-Cyclopentyl-2-hexadecylcyclopentane	$C_{26}H_{50}$	[C@H]1(CCC[C@@H]1CCCCCCCCCCCCCCCC)C1CCCC1	1
16	1-n-Hexadecylindan	$C_{25}H_{42}$	c1cccc2c1CC[C@H]2CCCCCCCCCCCCCCCC	1
18	1-Phenyl-3(2-Pheoylethyl)-hendecane	$C_{25}H_{36}$	c1ccc(cc1)CCC(CCc1ccccc1)CCCCCCCC	3
19	1-Cyclohexyl-3(2-cyclohexylethyl)hendecane	$C_{25}H_{48}$	C1CCC(CC1)CCC(CCCCCCCC)CCC1CCCCC1	1
22	6,11-di-n-amylhexadecane	$C_{26}H_{54}$	CCCCCC(CCCCC(CCCCC)CCCCC)CCCCC	3
23	3-ethyl-5(2-ethylbutyl)octadecane	$C_{26}H_{54}$	C(CCCCCCCCCCCCC)(CC(CC)CC)CC(CC)CC	1
25	9-n-octylheptadecane	$C_{25}H_{52}$	CCCCCCCCC(CCCCCCCC)CCCCCCCC	1
26	9-n-octyl-8-heptadecene	$C_{25}H_{50}$	CCCCCCCC=C(CCCCCCCC)CCCCCCCC	1
27	11-n-amylheneicosane	$C_{26}H_{54}$	CCCCCCCCCCC(CCCCCCCCCC)CCCCC	1
51	7-n-hexyleicosane	$C_{26}H_{54}$	CCCCCCC(CCCCCCCCCCCCC)CCCCCC	1
52	11-Phenyl-10-heneicosene	$C_{27}H_{46}$	c1ccccc1/C(=C\CCCCCCCCC)/CCCCCCCCCC	2
53	11(3-pentyl)heneicosane	$C_{26}H_{54}$	CCCCCCCCCCC(CCCCCCCCCC)C(CC)CC	1

54	11-Benzylheneicosane	$C_{28}H_{50}$	c1ccccc1CC(CCCCCCCCCC)CCCCCCCCCC	1
55	5,14-di-n-butyloctadecane	$C_{26}H_{54}$	CCCCC(CCCCCCCCC(CCCC)CCCC)CCCC	1
58	17-hexadecyltetratriacontane	$C_{50}H_{102}$	CCCCCCCCCCCCCCCCCC(CCCCCCCCCCCCCCCCC)CCCCCCCCCCCCCCCCC	1
59	11-20-di-n-decyltriacontane	$C_{50}H_{102}$	CCCCCCCCCCC(CCCCCCCCC(CCCCCCCCCC)CCCCCCCCCC)CCCCCCCCCC	3
60	11-Cyclohexylheneicosane	$C_{27}H_{54}$	C1CCCC(C1)C(CCCCCCCCCC)CCCCCCCCCC	1
61	11-alpha-Naphthyl-10-heneicosene	$C_{31}H_{48}$	c1c2c(c(cc1)/C(=C/CCCCCCCCC)/CCCCCCCCCC)cccc2	3
62	11-alpha-De-calylheneicosane	$C_{31}H_{60}$	C1[C@H]2[C@@H]([C@@H](CC1)C(CCCCCCCCCC)CCCCCCCCCC)CCCC2	1
63	9-n-octyleicosane	$C_{28}H_{58}$	CCCCCCCCC(CCCCCCCCCC)CCCCCCCC	1
64	11-Cyclopentyl-heneicosane	$C_{26}H_{52}$	C1(CCCC1)C(CCCCCCCCC)CCCCCCCCC	1
65	1-Cyclohexyl-2(cyclohexyl-methyl)pentadecane	$C_{28}H_{54}$	C1CCC(CC1)CC(CCCCCCCCCCCC)CC1CCCCC1	1
67	11-neopentylheneicosane	$C_{26}H_{54}$	CCCCCCCCCC(CCCCCCCCC)CC(C)(C)C	1
68	13-Phenylpentacosane	$C_{31}H_{56}$	c1ccccc1C(CCCCCCCCCCC)CCCCCCCCCCC	1
69	13-Cyclohexylpentacosane	$C_{31}H_{62}$	C1CCCC(C1)C(CCCCCCCCCCC)CCCCCCCCCCC	1
74	11-Cyclopentylmethylheneicosane	$C_{27}H_{54}$	C1(CCCC1)CC(CCCCCCCCC)CCCCCCCCC	2
75	3-Cyclohexyleicosane	$C_{26}H_{52}$	C1CCCC(C1)[C@H](CC)CCCCCCCCCCCCCCC	1
76	5-Cyclohexyleicosane	$C_{26}H_{52}$	C1CCCCC1[C@@H](CCCC)CCCCCCCCCCCCCC	3
77	7-Cyclohexyleicosane	$C_{26}H_{52}$	C1CCCCC1[C@@H](CCCCCC)CCCCCCCCCCC	2
78	9-Cyclohexyleicosane	$C_{26}H_{52}$	C1CCCCC1[C@@H](CCCCCCC)CCCCCCCCCC	1
79	3-Phenyleicosane	$C_{26}H_{46}$	c1cccc(c1)[C@@H](CC)CCCCCCCCCCCCCCC	1
80	5-Phenyleicosane	$C_{26}H_{46}$	c1cccc(c1)[C@@H](CCCC)CCCCCCCCCCCCC	1
81	7-Phenyleicosane	$C_{26}H_{46}$	c1cccc(c1)[C@H](CCCCCCCCCCCC)CCCCCC	1
82	9-Phenyleicosane	$C_{26}H_{46}$	c1cccc(c1)[C@H](CCCCCCCCCC)CCCCCCC	1
87	9(2-Phenylethyl)heptadecane	$C_{25}H_{44}$	c1cccc(c1)CCC(CCCCCCC)CCCCCCC	1
88	9(2-Cyclohexylethyl)heptadecane	$C_{25}H_{50}$	C1CCCC(C1)CCC(CCCCCCC)CCCCCCC	1
89	1,5-Diphenyl-3(2-pheoylethyl)pentane	$C_{25}H_{28}$	c1ccc(cc1)CCC(CCc1ccccc1)CCc1ccccc1	1
90	1,5-Dicyclohexyl-3(2-cyclopentylpropyl)pentane	$C_{25}H_{46}$	C1CCC(CC1)CCC(CCC1CCCCC1)CCC1CCCCC1	1
91	11-Cyclohexylmethylheneicosane	$C_{28}H_{56}$	C1CCCC(C1)CC(CCCCCCCCC)CCCCCCCCC	3
99	1-Phenyleicosane	$C_{26}H_{46}$	c1ccc(cc1)CCCCCCCCCCCCCCCCCC	1
100	1-Cyclohexyleicosane	$C_{26}H_{52}$	C1CCC(CC1)CCCCCCCCCCCCCCCCCC	1
101	2-Phenyleicosane	$C_{26}H_{46}$	c1ccccc1[C@@H](C)CCCCCCCCCCCCCCCC	1
102	2-Cyclohexyleicosane	$C_{26}H_{52}$	C1CCCC(C1)[C@H](CCCCCCCCCCCCCCCC)C	1
103	4-Phenyleicosane	$C_{26}H_{46}$	c1ccccc1[C@@H](CCC)CCCCCCCCCCCCCC	3
104	4-Cyclohexyleicosane	$C_{26}H_{52}$	C1CCCCC1[C@@H](CCC)CCCCCCCCCCCCCC	1
106	n-Hexacosane	$C_{26}H_{54}$	CCCCCCCCCCCCCCCCCCCCCCCCC	2
107	11-n-decyltetracosane	$C_{34}H_{70}$	CCCCCCCCCCC(CCCCCCCCCCCC)CCCCCCCCC	2
108	1-n-Hexadecyloctahydrindan	$C_{25}H_{48}$	C1[C@H]2[C@@H](CCC1)[C@H](CC2)CCCCCCCCCCCCCCC	1
109	3-ethyltetracosane	$C_{26}H_{54}$	CCC(CCCCCCCCCCCCCCCCCCCC)CC	1
110	9(3-Cyclopentylpropyl-heptadecane	$C_{25}H_{50}$	C1(CCCC1)CCCC(CCCCCCC)CCCCCCC	1
111	1-Cyclopentyl-4(3-cyclopentylpropyl)dodecane	$C_{25}H_{48}$	C1(CCCC1)CCCC(CCCC1CCCC1)CCCCCCC	1
112	1,7-Dicyclopentyl-4(3-cyclopentylpropyl)3-heptene	$C_{25}H_{44}$	C1CCC(C1)CCCC(=CCCC1CCCC1)CCCC1CCCC1	3
113	1,7-Dicyclopentyl-4(3-cyclopentylpropyl)heptane	$C_{25}H_{46}$	C(CCCC1CCCC1)(CCCC1CCCC1)CCCC1CCCC1	1
115	1,5-Dicyclopentyl-3(2-cyclopentylethyl) 2-pentene	$C_{25}H_{44}$	C1CCC(CC1)CCC(=CCC1CCCCC1)CCC1CCCCC1	1
116	1,1-Di-p-tolyldo-decane	$C_{26}H_{38}$	c1(ccc(cc1)C(c1ccc(cc1)C)CCCCCCCCCCC)C	1
117	1-Cyclopentyl-henelcosane	$C_{26}H_{52}$	C1(CCCC1)CCCCCCCCCCCCCCCCCCCC	2
118	2-n-Hexadecylhydrindan	$C_{25}H_{48}$	C1[C@H]2[C@@H](CCC1)C[C@H](C2)CCCCCCCCCCCCCCC	1

119	1,5-Dipthenyl-3(2-Phenylethyl-2-pentene	$C_{25}H_{26}$	c1ccc(cc1)CCC(=CCc1ccccc1)CCc1ccccc1	1
120	2-n-Hexadecylindan	$C_{25}H_{42}$	c1cccc2c1CC(C2)CCCCCCCCCCCCCCCC	1
121	1,10-Di(alphanaphthyl)l-hendecene	$C_{31}H_{34}$	c1cccc2c1cccc2C(=CCCCCCCCCC)c1c2ccccc2ccc1	1
122	1,1-Di(alpha-decalyl)-hendecane	$C_{31}H_{56}$	C1[C@H]2[C@@H]([C@@H](CC1)[C@H]([C@@H]1[C@H]3[C@@H](CCC1)CC CC3)CCCCCCCCCC)CCCC2	1
124	9-n-Dodecyclanthracene	$C_{26}H_{34}$	c1c2c(ccc1)c(c1c(c2)cccc1)CCCCCCCCCCCC	2
125	9-n-Dodecylperhydroanthracene	$C_{26}H_{48}$	C1[C@H]2[C@@H]([C@@H]([C@H]3[C@@H]1CCCC3)CCCCCCCCCCCC)CCCC2	1
126	1,5-Diphenyl-3(3-cyclopentylpropyl)pentane	$C_{25}H_{34}$	c1ccc(cc1)CCC(CCCC1CCCC1)CCc1ccccc1	3
127	1,5-Dicyclohexyl-3(3-cyclopentylpropyl)pentane	$C_{25}H_{46}$	C1CCC(CC1)CCC(CCCC1CCCC1)CCC1CCCCC1	1
128	1,7-Dicyclopentyl-4(2-phenylethyl)heptane	$C_{25}H_{40}$	c1(ccccc1)CCC(CCCC1CCCC1)CCCC1CCCC1	1
129	1,7-Dicyclopentyl-4(2-phenylethyl)heptane	$C_{25}H_{46}$	C1(CCCCC1)CCC(CCCC1CCCC1)CCCC1CCCC1	1
130	1-Phenyl-3(2-cyclohexylethyl)-6-cyclopentylhexane	$C_{25}H_{40}$	c1ccc(cc1)CC[C@H](CCC1CCCCC1)CCCC1CCCC1	1
131	1,10-Di(alphanaphthyl)decane	$C_{30}H_{34}$	c1cccc2c1cccc2CCCCCCCCCCc1c2ccccc2ccc1	2
132	1,10-Di(alphadecalyl)decane	$C_{30}H_{54}$	C1[C@H]2[C@@H]([C@@H](CC1)CCCCCCCCCC[C@@H]1CCC[C@@H]3[C@ @H]1CCCC3)CCCC2	1
133	13-n-undecylhexacosane	$C_{36}H_{74}$	CCCCCCCCCCCCC(CCCCCCCCCCCC)CCCCCCCCCC	1
134	13-n-dodecylhexacosane	$C_{38}H_{78}$	CCCCCCCCCCCCC(CCCCCCCCCCCCC)CCCCCCCCCC	1
135	15-Phenynonacosane	$C_{35}H_{64}$	c1ccccc1C(CCCCCCCCCCCCC)CCCCCCCCCCCC	1
136	15-Cyclohexylnomacosane	$C_{35}H_{70}$	C1CCCC(C1)C(CCCCCCCCCCCCC)CCCCCCCCCCCC	3
137	17-Phenyltritriacontane	$C_{39}H_{72}$	c1ccccc1C(CCCCCCCCCCCCCCC)CCCCCCCCCCCCC	1
138	17-Cyclohexyltritriacontane	$C_{39}H_{78}$	C1CCCC(C1)C(CCCCCCCCCCCCCCC)CCCCCCCCCCCCC	1
139	1,1-Di(4-methylcyclohexyl)dodecane	$C_{26}H_{50}$	[C@H]1(CC[C@@H](CC1)[C@@H](CCCCCCCCCC)[C@H]1CCC[C@H](C1)C)C	1
140	9-n-dodecyclphenanthrene	$C_{26}H_{34}$	c1c2c(ccc1)c1c(c(c2)CCCCCCCCCCC)cccc1	1
141	9-n-Dodecylperhydrophenanthrene	$C_{26}H_{48}$	C1[C@H]2[C@@H]([C@H]3[C@@H]([C@@H]1CCCCCCCCCCC)CCCC3)CCCC2	1
142	2-n-Dodecyl-9,10-dihydrophenanthrene	$C_{26}H_{36}$	c1cc2c(-c3c(cc(cc3)CCCCCCCCCCC)CC2)cc1	1
143	2-n-Dodecylperhydrophenanthrene	$C_{26}H_{48}$	C1[C@H]2[C@@H]([C@H]3[C@@H](C1)C[C@H](CC3)CCCCCCCCCCC)CCCC2	1
144	1,10-Di(5-indanyl)decane	$C_{28}H_{38}$	c12c(ccc(c1)CCCCCCCCCCc1ccc3c(c1)CCC3)CCC2	2
145	1,10-Di(5-hydrindanyl)decane	$C_{28}H_{50}$	[C@@H]12[C@@H](C[C@@H](CC1)CCCCCCCCCC[C@@H]1C[C@H]3[C@@H] (CC1)CCC3)CCC2	1
146	2-n-Dodecylphenanthrene	$C_{26}H_{34}$	c1c2c(ccc1)c1c(cc2)cc(cc1)CCCCCCCCCCC	1
152	1, 4-Di-n-decylbenzene	$C_{26}H_{46}$	c1(ccc(cc1)CCCCCCCCCC)CCCCCCCCCC	1
153	1,4-Di-n-decylcyclohexane	$C_{26}H_{52}$	[C@H]1(CC[C@@H](CC1)CCCCCCCCCC)CCCCCCCCCC	1
155	Cholestane	$C_{27}H_{48}$	C1[C@H]2[C@@](CCC1)([C@H]1[C@@H](CC2)[C@H]2[C@](CC1)([C@@H](CC2) [C@H](C)CCCC(C)C)C)C	2
156	2,4,6-Trimethyln-octadecylbenzene	$C_{27}H_{48}$	c1(cc(c(c(c1)C)CCCCCCCCCCCCCCCCCC)C)C	1
157	1,4,5-Trimethyl-n-octadecylcyclohexane	$C_{27}H_{54}$	[C@H]1(C[C@@H]([C@@H]([C@@H](C1)C)CCCCCCCCCCCCCCCCCC)C)C	2
158	2,5-Dimethyln-octadecylbenzene	$C_{26}H_{46}$	c1cc(c(cc1C)CCCCCCCCCCCCCCCCCC)C	2
159	2,5-Dimethyl-n-octadecylcyclohexane	$C_{26}H_{52}$	C1C[C@@H]([C@@H](C[C@@H]1C)CCCCCCCCCCCCCCCCCC)C	3
161	8-p-Tolylnonadecane	$C_{26}H_{46}$	c1cc(ccc1[C@H](CCCCCCCCCC)CCCCCCC)C	3
162	8(4-Methylcyclohexyl)nonadecane	$C_{26}H_{52}$	[C@H]1(CC[C@@H](CC1)[C@@H](CCCCCCC)CCCCCCCCCC)C	1
163	9-n-hexylheptadecane	$C_{23}H_{48}$	CCCCCCCCC(CCCCCCCC)CCCCCC	1
164	9-n-octylhexacosane	$C_{34}H_{70}$	CCCCCCCCC(CCCCCCCCCCCCCCCC)CCCCCCCC	1
165	1,2,3,4,5,6,7,8,9,10,17,18-Dodecahydro-9(n-octyl)naphthacene	$C_{26}H_{40}$	c1c2c(cc3c1C[C@@H]1[C@H]([C@H]3CCCCCCCC)CCCC1)CCCC2	1
166	9-n-Octylperhydronaphthacene	$C_{26}H_{46}$	C1[C@H]2[C@@H](C[C@H]3[C@H]1CCCC3)[C@H]([C@@H]1[C@H](C2) CCCC1)CCCCCCCC	1
167	11(2,5-Dimethylphenyl)10-heneicosene	$C_{29}H_{50}$	c1cc(c(cc1C)/C(=C/CCCCCCCCC)/CCCCCCCCCC)C	1
168	11(2,5-Dimethylphenyl)heneicosane	$C_{29}H_{52}$	c1cc(c(cc1C)C(CCCCCCCCCC)CCCCCCCCCC)C	2
169	11(2,5-Dimethylcyclohexyl)heneicosane	$C_{29}H_{58}$	[C@H]1(CC[C@@H]([C@@H](C1)C(CCCCCCCCCC)CCCCCCCCCC)C)C	2

170	1,7-Diphenyl-4(3-phenylpropyl)3-heptane	$C_{28}H_{32}$	c1ccc(cc1)CCCC(=CCCc1ccccc1)CCCc1ccccc1	2
171	1,7-Diphenyl-4(3-phenylpropyl)heptane	$C_{28}H_{34}$	c1ccc(cc1)CCCC(CCCc1ccccc1)CCCc1ccccc1	1
172	1,7-Dicyclohexyl-4(3-cyclohexylpropyl)heptane	$C_{28}H_{52}$	C1CCC(CC1)CCCC(CCCC1CCCCC1)CCCC1CCCCC1	2
173	11-alpha-ar-Tetralylheneicosane	$C_{31}H_{54}$	c1c2c(c(cc1)C(CCCCCCCCCC)CCCCCCCCCC)CCCC2	1
174	1-alpha-Naphthylpentadecane	$C_{25}H_{38}$	c1c2c(c(cc1)CCCCCCCCCCCCCCC)cccc2	1
175	1-alpha-Decalylpentadecane	$C_{25}H_{48}$	C1[C@H]2[C@@H](CCC1)[C@@H](CCC2)CCCCCCCCCCCCCCC	1
176	n-Octacosane	$C_{28}H_{58}$	CCCCCCCCCCCCCCCCCCCCCCCCCCCC	1
177	9(4-as-perhydroindacenyl)heptadecane	$C_{29}H_{54}$	[C@@H]12[C@H]3[C@@H]([C@@H](C[C@@H]1CCC2)C(CCCCCCCC)CCCCCCCC)CCC3	1
178	9(alpha(cis-0,3,3-Bi-cyclooctyl-methyllheptadecane	$C_{26}H_{50}$	[C@H]1([C@H]2[C@@H](CC1)CCC2)CC(CCCCCCCC)CCCCCCCC	1
179	9-n-Octyl(1,2,3,4-tetrahydro)naphthacene	$C_{26}H_{32}$	c1c2c(cc3c1CCCC3)c(c1c(c2)cccc1)CCCCCCCC	1
180	11(2,4-Dimethyleyclopentylmethyl)beneicosane	$C_{29}H_{58}$	[C@H]1(C[C@H](C[C@@H]1C)C)CC(CCCCCCCCCC)CCCCCCCCCC	2
181	9(5-Exo-perhydro-4,7-methanoindenylmethyl)-heptadecane	$C_{28}H_{52}$	[C@@H]12[C@@H]3[C@H]([C@@H]([C@@H](C1)CC(CCCCCCCC)CCCCCCC)C2)CCC3	1
182	2,2,4,15,17,17-hexamethyl-7,12-di(3,5,5-trimethylhexyl)octadecane	$C_{42}H_{86}$	[C@H](CCCC[C@@H](CC[C@H](CC(C)(C)C)C)CC[C@H](CC(C)(C)C)C)(CC[C@H](CC(C)(C)C)C)CC[C@@H](CC(C)(C)C)C	1
183	2,2,4,10,12,12-hexamethyl-7(3,5,5-trimethylhexyl)-6-tridecene	$C_{28}H_{56}$	C(=C\C[C@@H](CC(C)(C)C)C)(\CC[C@@H](CC(C)(C)C)C)/CC[C@H](CC(C)(C)C)C	1
184	2,2,4,10,12,12-hexamethyl-7(3,5,5-trimethylhexyl)tridecane	$C_{28}H_{58}$	C(CC[C@H](CC(C)(C)C)C)(CC[C@H](CC(C)(C)C)C)CC[C@H](CC(C)(C)C)C	1
188	1(1-ar-Tetralyl)pentadecane	$C_{25}H_{42}$	c1c2c(c(cc1)CCCCCCCCCCCCCCC)CCCC2	2
189	1(5-Acenaphthyl)pentadecane	$C_{27}H_{40}$	c12c3c(c(cc1)CCCCCCCCCCCCCCC)cccc3CC2	1
190	n-Hexatriacontane	$C_{36}H_{74}$	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	1
191	9-n-octyltetracosane	$C_{32}H_{66}$	CCCCCCCCC(CCCCCCCCCCCCCCC)CCCCCCCC	1
192	1-Cyclohexyl-4(alpha-de-calyl)tetradecane	$C_{30}H_{56}$	C1[C@H]2[C@@H](CCC1)[C@@H](CCC2)[C@H](CCCCCCCCCC)CCCC1CCCCC1	2
193	1(5-Perhydro-acenaphthyl-pentadecane	$C_{27}H_{50}$	[C@@H]12[C@H]3[C@@H]([C@@H](CC1)CCCCCCCCCCCCCCC)CCC[C@H]3CC2	2
196	6-n-Octylperhydrobenz(de)-anthracene	$C_{25}H_{44}$	C1[C@H]2[C@@H](CCC1)C[C@H]1[C@H](CC[C@@H]3[C@H]1[C@@H]2CCC3)CCCCCCCC	2
197	n-Dotriacontane	$C_{32}H_{66}$	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	1
199	1,3-Dicyclopentyl-2-dodecylcyclopentane	$C_{27}H_{50}$	[C@H]1([C@@H](CC[C@@H]1C1CCCC1)C1CCCC1)CCCCCCCCCCCC	1
200	1,1-Di(5-perhydroxcenaphthyl)ethane	$C_{26}H_{42}$	[C@@H]12[C@H]3[C@@H](CCC1)[C@@H](CC[C@@H]3CC2)[C@H]([C@@H]1[C@H]2CCC[C@@H]3[C@H]2[C@@H](CC1)CC3)C	1
202	1,1-Dicyclopentylhexadecane	$C_{26}H_{50}$	CCCCCCCCCCCCCCCC(C1CCCC1)C1CCCC1	1
203	tri(alphadecalyl)methane	$C_{31}H_{52}$	C1[C@H]2[C@@H](CCC1)[C@@H](CCC2)[C@@H]([C@@H]1CCC[C@@H]2[C@H]1CCCC2)[C@H]1CCC[C@H]2[C@@H]1CCCC2	1
204	13(alpha-Decalyl)-perhydrodibenzo-(a,i)-fluorene	$C_{31}H_{50}$	[C@@H]12[C@@H]([C@H]3[C@@H]([C@@H]1[C@H]1CCC[C@@H]4[C@@H]1CCCC4)[C@@H]1[C@H](CC3)CCCC1)CC[C@@H]1[C@H]2CCCC1	1
205	n-Tetratetracontane	$C_{44}H_{90}$	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	1
206	1,4-Di(4-phenylbutyl)benzene	$C_{26}H_{30}$	c1ccc(cc1)CCCCc1ccc(cc1)CCCCc1ccccc1	1
207	1,4-Di(4-cyclohexylbutyl)cyclohexane	$C_{26}H_{48}$	[C@@H]1(CC[C@@H](CC1)CCCCC1CCCCC1)CCCCC1CCCCC1	3
208	1,3-Di-n-decylbenzene	$C_{26}H_{46}$	c1cc(cc(c1)CCCCCCCCCC)CCCCCCCCCC	1
209	1,3-Di-n-decylcyclohexane	$C_{26}H_{52}$	[C@H]1(CCC[C@@H](C1)CCCCCCCCCC)CCCCCCCCCC	3
210	9-ethyl-9-n-heptyloctadecane	$C_{27}H_{56}$	CCCCCCCC[C@](CCCCCCCCC)(CC)CCCCCCC	1
211	10-n-heptyl-10-n-octyleicosane	$C_{35}H_{72}$	CCCCCCCCC[C@](CCCCCCCCCC)(CCCCCCC)CCCCCCCC	1
215	3-n-Decylpyrene	$C_{26}H_{30}$	c1cc2c3c(c1CCCCCCCCCC)ccc1c3c(ccc1)cc2	1
216	3-n-Decylperhydropyrene	$C_{26}H_{46}$	[C@H]12[C@H]3[C@H]4[C@H](CC1)CC[C@H]([C@@H]4CC[C@@H]3CCC2)CCCCCCCCCC	2
218	1-n-Decyl-3,4,5,8,9,10-hexahydropyrene	$C_{26}H_{36}$	c12c3c4c(cc1)CCCc4c(cc3CCC2)CCCCCCCCCC	1
219	4-Decylperhydropyrene*	$C_{26}H_{46}$	[C@H]12[C@H]3[C@H]4[C@H](CC1)CCC[C@@H]4[C@H](C[C@@H]3CCC2)CCCCCCCCCC	1
220	n-Pentatriacontane	$C_{35}H_{72}$	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	3
223	2,6,10,15,19,23-hexamethyltetracosane	$C_{30}H_{62}$	CC(CCC[C@@H](CCC[C@@H](CCCC[C@H](CCC[C@H](CCCC(C)C)C)C)C)C)C	1

224	2-n-Octylchrysene	$C_{26}H_{28}$	c1cc2c(cc1)c1c(c3c(c(c1)CCCCCCCC)cccc3)cc2	3
225	2-Octylperhydrochrysene	$C_{26}H_{46}$	C1[C@H]2[C@@H](CCC1)[C@H]1[C@H](CC2)[C@@H]2[C@@H]([C@@H](C1)CCCCCCCC)CCCC2	2
226	2-Octyltriphenylene*	$C_{26}H_{28}$	c1cc2c(cc1)c1c(c3cc(ccc23)CCCCCCCC)cccc1	3
228	2-Octylperhydrotriphenylene*	$C_{26}H_{46}$	C1[C@H]2[C@@H](CCC1)[C@H]1[C@H]([C@@H]3[C@H]2CC[C@@H](C3)CCCCCCCC)CCCC1	3
229	7-Hexadecylspiro(4,5)decane	$C_{26}H_{50}$	C1CCC2(C[C@@H]1CCCCCCCCCCCCCCCC)CCCC2	1
230	2-Decyl-4b,5,9b,10-tetrahydroindeno(2.1-a)indene*	$C_{26}H_{34}$	c1c2c(ccc1)C[C@H]1[C@@H]2Cc2ccc(cc12)CCCCCCCCCC	2
231	2-Decylperhydroindeno(2.1-a)-indene*	$C_{26}H_{46}$	C1[C@H]2[C@@H](CCC1)C[C@@H]1[C@@H]2C[C@@H]2CC[C@@H](C[C@H]12)CCCCCCCCCC	1
232	11-Octyl-1,2,3,4,5,6,7,8,13,14,15,16-decahydrochrynene*	$C_{26}H_{40}$	c12c(c3c(c(c1)CCCCCCCC)CCCC3)CC[C@@H]1[C@@H]2CCCC1	1
235	1,4-Dimethyl-2-(3,7-Dimethyl-octyl) benzene	$C_{18}H_{30}$	c1cc(c(cc1C)CC[C@@H](CCCC(C)C)C)C	2
236	9-n-Dodecylfluorene*	$C_{25}H_{34}$	c1cccc2c1-c1c(C2CCCCCCCCCCCC)cccc1	1
237	Perhydro-9-n-dodecylfluorene*	$C_{25}H_{46}$	C1[C@@H]2[C@@H](CCC1)[C@H]([C@H]1CCCC[C@@H]21)CCCCCCCCCCCC	3
500	7-n-hexyltridecane	$C_{19}H_{40}$	CCCCCCC(CCCCCC)CCCCCC	1
501	1, 1-Diphenyl-1-heptene	$C_{19}H_{22}$	c1ccc(cc1)C(=CCCCCC)c1ccccc1	1
502	7-Phenyltri-decane	$C_{19}H_{32}$	c1ccc(cc1)C(CCCCCC)CCCCCC	1
503	1, 1-Diphenyl-heptene	$C_{19}H_{24}$	c1ccc(cc1)C(c1ccccc1)CCCCCC	1
504	7-Cyclohexyltridecane	$C_{19}H_{38}$	C1CCC(CC1)C(CCCCCC)CCCCCC	1
505	1,1-Dicyclohexylheptane	$C_{19}H_{36}$	C1CCC(CC1)C(CCCCCC)C1CCCCC1	1
506	7-Phenyl-6-tridecene	$C_{19}H_{30}$	c1ccc(cc1)/C(=C/CCCCC)/CCCCCC	1
507	Tricyclohexylmethane	$C_{19}H_{34}$	C1CCC(CC1)C(C1CCCCC1)C1CCCCC1	1
509	9-Cyclohexyl-heptadecane	$C_{23}H_{46}$	C1CCC(CC1)C(CCCCCCCC)CCCCCCCC	1
510	4-n-propylheptadecane	$C_{20}H_{42}$	CCCC(CCCCCCCCCCCCC)CCC	1
511	5-n-butylhexadecane	$C_{20}H_{42}$	CCCCC(CCCCCCCCCCC)CCCC	1
512	7-methyltridecane	$C_{14}H_{30}$	CCCCCCC(CCCCCC)C	1
513	2-Phenyloctane	$C_{14}H_{22}$	c1cccc(c1)[C@H](CCCCCC)C	2
514	2-cyclohexyloctane	$C_{14}H_{28}$	C1CCC(CC1)[C@@H](C)CCCCCC	1
516	1,1-Diphenyl-ethane	$C_{14}H_{14}$	c1ccc(cc1)C(c1ccccc1)C	3
517	1-Phenyl-1-cyclohexylethane	$C_{14}H_{20}$	c1ccc(cc1)[C@@H](C1CCCCC1)C	1
518	1,1-Dicyclohexylethane	$C_{14}H_{26}$	C1CCC(CC1)C(C)C1CCCCC1	1
519	1,2-Diphenyl-ethane	$C_{14}H_{14}$	c1ccc(cc1)CCc1ccccc1	1
520	1,2-Dicyclohexylethane	$C_{14}H_{26}$	C1CCC(CC1)CCC1CCCCC1	1
521	1-Phenyl-2-cyclohexylethane	$C_{14}H_{20}$	c1ccc(cc1)CCC1CCCCC1	1
522	1-Phenyl-3-cyclopentylpropane	$C_{14}H_{20}$	c1ccc(cc1)CCCC1CCCC1	1
523	1-Cyclohexyl-3-cyclopentylpropane	$C_{14}H_{26}$	C1CCC(CC1)CCCC1CCCC1	1
524	diphenylmethane	$C_{13}H_{12}$	c1ccc(cc1)Cc1ccccc1	1
525	Dicyclohexylmethane	$C_{13}H_{24}$	C1CCC(CC1)CC1CCCCC1	3
526	9-n-Butylanthracene	$C_{18}H_{18}$	c1cc2c(cc1)c(c1c(c2)cccc1)CCCC	2
527	9-n-Butylperhydroanthracene	$C_{18}H_{32}$	C1[C@H]2[C@@H](CCC1)[C@H]([C@@H]1[C@H](C2)CCCC1)CCCC	3
528	n-Dodecane	$C_{12}H_{26}$	CCCCCCCCCCCC	1
529	n-Tridecane	$C_{13}H_{28}$	CCCCCCCCCCCCC	1
530	1-Tridecene	$C_{13}H_{26}$	C=CCCCCCCCCCC	1
531	n-Tetradecane	$C_{14}H_{30}$	CCCCCCCCCCCCCC	1
532	n-Pentadecane	$C_{15}H_{32}$	CCCCCCCCCCCCCCC	1
533	1-Pentadecene	$C_{15}H_{30}$	C=CCCCCCCCCCCCC	1
534	n-Hexadecane	$C_{16}H_{34}$	CCCCCCCCCCCCCCCC	1
535	n-Heptadecane	$C_{17}H_{36}$	CCCCCCCCCCCCCCCCC	1
536	1-Heptadecene	$C_{17}H_{34}$	C=CCCCCCCCCCCCCCC	1

537	n-Octadecane	$C_{18}H_{38}$	CCCCCCCCCCCCCCCCCC	3
538	1-Phenyloctane	$C_{14}H_{22}$	c1ccc(cc1)CCCCCCCC	1
539	1-cyclohexyloctane	$C_{14}H_{28}$	C1CCC(CC1)CCCCCCCC	1
540	n-Eicosane	$C_{20}H_{42}$	CCCCCCCCCCCCCCCCCCCC	1
541	n-Tetracosane	$C_{24}H_{50}$	CCCCCCCCCCCCCCCCCCCCCCCC	1
542	7-Cyclopentylmethyltridecane	$C_{19}H_{38}$	C1CCC(C1)CC(CCCCCC)CCCCCC	1
543	cis(0,3,3)Bicyclo-octane	C_8H_{14}	C1[C@H]2[C@@H](CC1)CCC2	1
544	1-alpha-Decalylhendecane	$C_{21}H_{40}$	C1[C@H]2[C@@H]([C@@H](CC1)CCCCCCCCCCC)CCCC2	1
545	7-n-propyltridecane	$C_{16}H_{34}$	CCCCCCC(CCCCCC)CCC	3
546	5-n-butylnonane	$C_{13}H_{28}$	CCCCC(CCCC)CCCC	3
547	5-n-butyl-4-nonene	$C_{13}H_{26}$	CCC/C(=C/CCCC)/CCCC	1
548	1,3-Dicyclopentylcyclopentane	$C_{15}H_{26}$	C1CCC(C1)[C@H]1CC[C@@H](C1)C1CCCC1	1
549	4-n-propylheptane	$C_{10}H_{22}$	CCCC(CCC)CCC	1
550	4-n-propyl-3-heptene	$C_{10}H_{20}$	CCC=C(CCC)CCC	3
551	Bicyclopentyl	$C_{10}H_{18}$	C1C(CCC1)C1CCCC1	1
552	1,5-Dicyclopentyl-3(2-cyclopentylethyl) 2-pentene	$C_{22}H_{38}$	C1CC(CC1)CCC(=CCC1CCCC1)CCC1CCCC1	2
553	1,5-Dicyclopentyl-3(2-cyclopentylethyl) 2-pentene	$C_{22}H_{40}$	C(CCC1CCCC1)(CCC1CCCC1)CCC1CCCC1	1
554	8-n-hexylpentadecane	$C_{21}H_{44}$	CCCCCCCC(CCCCCCC)CCCCCC	1
555	2,2,3,5,5,6,6-heptamethyl-3-heptene	$C_{14}H_{28}$	CC(/C(=C/C(C(C)(C)C)(C)C)/C)(C)C	3
556	2,2,3,3,5,6,6-heptamethylheptane	$C_{14}H_{30}$	CC([C@H](CC(C(C)(C)C)(C)C)C)(C)C	3
557	4-9-di-n-propyldodecane	$C_{18}H_{38}$	CCCC(CCCCC(CCC)CCC)CCC	3
559	1-alpha-Napthylbendecane	$C_{21}H_{30}$	c1c2c(ccc1)c(ccc2)CCCCCCCCCCC	1
560	1,1,-diphenylethylene	$C_{14}H_{12}$	c1ccc(cc1)/C=C/c1ccccc1	1
561	Perhydrofluorene	$C_{13}H_{22}$	C1[C@@H]2[C@@H](CCC1)C[C@H]1CCCC[C@@H]21	1
562	1,2-Di(alphadecalyl)ethane	$C_{22}H_{38}$	C1[C@@H]2[C@@H]([C@@H](CC1)CC[C@@H]1[C@H]3[C@@H](CCC1)CCCC3)CCCC2	3
563	1,1-Di(alphadecalyl)ethane	$C_{22}H_{38}$	C1[C@H]2[C@@H](CCC1)[C@@H](CCC2)[C@@H](C)[C@H]1[C@@H]2[C@@H](CCCC2)CCC1	2
564	Tricyclopentylmethane	$C_{16}H_{28}$	C1CCC(C1)C(C1CCCC1)C1CCCC1	2
565	1-Undecene	$C_{11}H_{22}$	C=CCCCCCCCCC	1
566	1-Dodecene	$C_{12}H_{24}$	C=CCCCCCCCCCC	1
567	1-Methylnaphthalene	$C_{11}H_{10}$	c1cc2c(cc1)c(ccc2)C	2
568	2-Methylnaphthalene	$C_{11}H_{10}$	c1cc2c(cc1)cc(cc2)C	1
569	cis-Decahydro-naphthalene	$C_{10}H_{18}$	C1[C@@H]2[C@@H](CCC1)CCCC2	1
570	trans-Decahydro-naphthalene	$C_{10}H_{18}$	C1[C@@H]2[C@@H](CCC1)CCCC2	1
571	1-Phenyldecane	$C_{16}H_{26}$	c1ccc(cc1)CCCCCCCCCC	2
572	1-Cyclohexyldecane	$C_{16}H_{32}$	C1CCC(CC1)CCCCCCCCCC	1
573	1-Cyclopentyldecane	$C_{15}H_{30}$	C1CCC(C1)CCCCCCCCCC	3
574	1 2,3,4,5,6,7,8,13,14,15,16-Dodecahydrochrysene	$C_{18}H_{24}$	c12c(c3c(cc1)CCCC3)CC[C@@H]1[C@H]2CCCC1	1
575	Perhydrochrysene	$C_{18}H_{30}$	C1[C@H]2[C@@H]([C@H]3[C@@H](C1)CC[C@@H]1[C@@H]3CCCC1)CCCC2	1
576	1,2,3,4-Tetrahydrofluoranthene	$C_{16}H_{14}$	c1cc2c3c(-c4c([C@@H]3CCC2)cccc4)c1	1
577	Perhydrofluoranthene	$C_{16}H_{26}$	C1[C@H]2[C@H]3[C@@H](CC1)[C@@H]1[C@H]([C@@H]3CCC2)CCCC1	1
578	Perhydropyrene	$C_{16}H_{26}$	C1C[C@H]2[C@H]3[C@@H](C1)CC[C@@H]1[C@@H]3[C@@H](CCC1)CC2	1
580	1,1-Dicyclopentylethane	$C_{12}H_{22}$	C1CC(CC1)C(C)C1CCCC1	2
581	2-methyldecane	$C_{11}H_{24}$	CC(CCCCCCCC)C	1
582	2-methylpentadecane	$C_{16}H_{34}$	CC(CCCCCCCCCCCCC)C	3
583	2-methylheptadecane	$C_{18}H_{38}$	CC(CCCCCCCCCCCCCCC)C	1
584	2-methyltricosane	$C_{24}H_{50}$	CC(CCCCCCCCCCCCCCCCCCCCC)C	2

586	Di(alpha -decalyl)-methane	$C_{21}H_{36}$	C1[C@H]2[C@@H](CCC1)[C@@H](CCC2)C[C@@H]1CCC[C@H]2[C@@H]1CCCC2	2
587	Perhydrodibenzo-(a,i)fluorene	$C_{21}H_{34}$	C1[C@@H]2[C@@H]([C@H]3[C@@H](C1)CCCC3)C[C@H]1[C@@H]3[C@H](CC[C@@H]21)CCCC3	3
588	3-methyleicosane	$C_{21}H_{44}$	CC[C@H](CCCCCCCCCCCCCCCCC)C	2
589	1-Tetradecene	$C_{14}H_{28}$	C=CCCCCCCCCCCCC	1
590	1-Hexadecene	$C_{16}H_{32}$	C=CCCCCCCCCCCCCCC	2
591	10-methyleicosane	$C_{21}H_{44}$	CCCCCCCCC[C@@H](CCCCCCCCCC)C	1
592	2(ar)-Butyltetralin	$C_{14}H_{20}$	c1cc2c(cc1CCCC)CCCC2	1
593	2(ar)-Decylitetralin	$C_{20}H_{32}$	c1c2c(cc(c1)CCCCCCCCCC)CCCC2	2
594	2-Decyldacalin	$C_{20}H_{38}$	C1[C@H]2[C@@H](C[C@@H](C1)CCCCCCCCCC)CCCC2	1
595	2-Decylindan	$C_{19}H_{30}$	c1cc2c(cc1)CC(C2)CCCCCCCCCC	1
596	2-Decylhydrindan	$C_{19}H_{36}$	C1[C@@H]2[C@@H](CCC1)C[C@H](C2)CCCCCCCCCC	1
597	5-Decylindan	$C_{19}H_{30}$	c1cc2c(cc1CCCCCCCCCC)CCC2	1
598	5-Decylhydrindan	$C_{19}H_{36}$	C1[C@@H]2[C@@H](C[C@@H](C1)CCCCCCCCCC)CCC2	1
599	2-Butyl-lhexylindene	$C_{19}H_{28}$	c1cc2c(cc1)C(=C(C2)CCCC)CCCCCC	1
600	2-Butyl-1-hexylindan	$C_{19}H_{30}$	c1cc2c(cc1)[C@@H]([C@H](C2)CCCC)CCCCCC	1
601	2-Butyl-l-hexylhydrindan	$C_{19}H_{36}$	C1[C@H]2[C@@H](CCC1)[C@H]([C@H](C2)CCCC)CCCCCC	3
602	2-Butyl-5-hexylindan	$C_{19}H_{30}$	c1cc2c(cc1CCCCCC)C[C@H](C2)CCCC	1
603	2-Butyl-5-hexylhydrindan	$C_{19}H_{36}$	C1[C@H]2[C@@H](C[C@@H](C1)CCCCCC)C[C@@H](C2)CCCC	1
604	5-Butyl-6-hexylindan	$C_{19}H_{30}$	c1(cc2c(cc1CCCC)CCC2)CCCCCC	2
605	5-Butyl-6-hexylindan	$C_{19}H_{36}$	C1[C@H]2[C@@H](C[C@@H]([C@@H]1CCCCCC)CCCC)CCC2	3
606	2-n-Butylnaphthalene	$C_{14}H_{16}$	c1cc2c(cc1CCCC)cccc2	3
607	2-n-Butyldecalin	$C_{14}H_{26}$	C1[C@H]2[C@@H](CCC1)C[C@H](CC2)CCCC	1
608	Bicyclohexyl	$C_{12}H_{22}$	C1C(CCCC1)C1CCCCC1	3
609	n-Nonadecane	$C_{19}H_{40}$	CCCCCCCCCCCCCCCCCCC	1
610	7-n-Butyl-l-n-hexyloaphthalene	$C_{20}H_{28}$	c1c2c(c(cc1)CCCCCC)cc(cc2)CCCC	1
611	7(ar)-n-Butyl-1-n-hexyltetralin	$C_{20}H_{32}$	c1c2c(cc(c1)CCCC)[C@H](CCC2)CCCCCC	3
612	7-n-Butyl-l-n-hexydecalin	$C_{20}H_{38}$	C1[C@H]2[C@@H]([C@@H](CC1)CCCCCC)C[C@H](CC2)CCCC	3
613	2-n-Butyl-3-n-hexyloaphthalene	$C_{20}H_{28}$	c1c2c(ccc1)cc(c(c2)CCCCCC)CCCC	1
614	2(ar)-n-Butyl-3(ar)-n-hexyltetralin	$C_{20}H_{32}$	c1c2c(cc(c1CCCC)CCCCCC)CCCC2	1
615	2-n-Butyl-3-n-hexyldecalin	$C_{20}H_{38}$	C1[C@H]2[C@@H](CCC1)C[C@H]([C@H](C2)CCCCCC)CCCC	1
616	4,5-Dimethylphenanthrene	$C_{16}H_{14}$	c1cc2c(c(c1)C)c1c(cc2)cccc1C	3
617	4,5-Dimethyl-9,10-dihydrophenanthrene	$C_{16}H_{16}$	c1cc2c(-c3c(CC2)cccc3C)c(c1)C	1
618	4,5-Dimethylperhydrophenanthrene	$C_{16}H_{28}$	C1C[C@H]2[C@@H]([C@@H](C1)C)[C@H]1[C@@H](CCC[C@@H]1C)CC2	2
619	n-Tricosane	$C_{23}H_{48}$	CCCCCCCCCCCCCCCCCCCCCCC	1
620	Spiro(4,5)decane	$C_{10}H_{18}$	C12(CCCC1)CCCCC2	1
622	Spiro(5,5)undecane	$C_{10}H_{20}$	C1CCC2(CC1)CCCCC2	1
623	Spiro(5,6)dodecane	$C_{12}H_{22}$	C1CCC2(CC1)CCCCCC2	1
625	1,2,3,4,5,6,7,8-Octahydrophenanthrene	$C_{14}H_{18}$	c1cc2c(c3c1CCCC3)CCCC2	2
626	Perhydrophenanthren	$C_{14}H_{24}$	C1[C@H]2[C@@H](CCC1)[C@H]1[C@H](CC2)CCCC1	1
627	2,6-Dimethy-3-octylnapthalene	$C_{20}H_{28}$	c1c2c(ccc1C)cc(c(c2)CCCCCCCC)C	1
628	2(ar),6-Dimethyl-3-octyltetralin	$C_{20}H_{32}$	c1c2c(cc(c1C)CCCCCCCC)C[C@H](CC2)C	1
629	2,6-Dimethyl-3-octyldecalin	$C_{20}H_{38}$	C1[C@H]2[C@@H](C[C@@H]([C@@H]1C)CCCCCCCC)C[C@H](CC2)C	1
631	1,3-Diphenyl-benzene	$C_{18}H_{14}$	c1ccc(cc1)c1cccc(c1)c1ccccc1	2
632	1,3-Dicyclopentylcyclopentane	$C_{18}H_{32}$	C1C[C@@H](C[C@@H](C1)C1CCCCC1)C1CCCCC1	1
633	1,2-Diphenyl-benzene	$C_{18}H_{14}$	c1ccc(cc1)c1ccccc1c1ccccc1	1
634	1,2-Dicyclohexylcyclohexane	$C_{18}H_{32}$	C1C[C@@H]([C@@H](CC1)C1CCCCC1)C1CCCCC1	1
637	Perhydroanthracene	$C_{14}H_{24}$	C1[C@H]2[C@@H](CCC1)C[C@H]1CCCC[C@H]1C2	1

638	1,4-Dimethyl-5-octylnaphthalene	$C_{20}H_{28}$	c1(c2c(c(cc1)C)c(ccc2)CCCCCCCC)C	1
639	1(ar),4-Dimethyl-5-octyltetralin	$C_{20}H_{32}$	c1(c2c(c(cc1)C)[C@H](CCC2)CCCCCCCC)C	1
640	1,4-Dimethyl-5-octyldecalin	$C_{20}H_{38}$	C1[C@H]2[C@@H]([C@@H](CC1)CCCCCCCC)[C@@H](CC[C@H]2C)C	1
641	1,2,2a,3,4,5-Hexahydropyrene	$C_{16}H_{16}$	c12c3c4c(cc1)cccc4CC[C@@H]3CCC2	2
642	2,6,10,14-tetramethylpentadecane	$C_{19}H_{40}$	CC(CCC[C@@H](CCC[C@@H](CCCC(C)C)C)C)C	1
643	2,6,11,15-tetramethylhexadecane	$C_{20}H_{42}$	CC(CCC[C@@H](CCCC[C@H](CCCC(C)C)C)C)C	1
645	Perhydroindeno(2,1-a)indene*	$C_{16}H_{26}$	C1C[C@@H]2[C@@H](CC1)C[C@H]1[C@H]2C[C@H]2CCCC[C@H]12	1
646	1-t-Butylnaphthalene	$C_{14}H_{16}$	c1cc2c(cc1)c(ccc2)C(C)(C)C	1
647	1-t-Butyldecahydronaphthalene*	$C_{14}H_{26}$	C1[C@H]2[C@@H](CCC1)[C@@H](CCC2)C(C)(C)C	3
648	1,2,3,4,4a,9,10,10a-Octahydro-3-hexly-6-butylphenanthrene*	$C_{24}H_{36}$	c1c2c(cc(c1)CCCC)[C@H]1[C@H](CC2)CC[C@@H](C1)CCCCCC	1
652	2-t-Butylnaphthalene	$C_{14}H_{16}$	c1cc2c(cc1)cc(cc2)C(C)(C)C	1
654	Perhydro-1,2,5,6-dibenzcyclo-octane*	$C_{16}H_{28}$	C1[C@H]2[C@@H](CCC1)CC[C@H]1CCCC[C@H]1CC2	1

Experimental Data

The experimental dynamic viscosity and density of all the 305 hydrocarbons are listed in Table S2 from 0 °C to 135 °C. For these molecules, the dynamic viscosity and density range from 0.29 cP to 2.00×10^4 cP and 0.67 g/cc to 1.12 g/cc, respectively.

Table S2: Experimental dynamic viscosity and density of the hydrocarbon molecules from API Project 42 [1].

PS U#	Dynamic Viscosity [cP]					Density [g/cc]				
	32	68	100	140	210	32	68	100	140	210
1	37.46	15.24	8.2	4.466	2.0930	0.8172	0.8041	0.7924	0.7780	0.7529
2	-	15.6	8.389	4.56	2.1200	0.8178	0.8043	0.7930	0.7785	0.7530
3	41.03	16.44	8.774	4.74	2.2000	0.8183	0.8042	0.7928	0.7784	0.7532
4	-	17.11	9.09	4.94	2.2800	0.8194	0.8059	0.7946	0.7796	0.7548
5	-	20.11	10.41	5.59	2.5100	0.8210	0.8080	0.7969	0.7820	0.7571
6	-	22.19	11.5	6.05	2.7000	0.8246	0.8114	0.7999	0.7855	0.7609
7	67.96	25.81	13.21	6.86	2.9800	0.8263	0.8129	0.8017	0.7876	0.7630
8	-	23.53	12.06	6.33	2.7900	0.8245	0.8117	0.8005	0.7862	0.7616
9	-	26.34	12.84	6.42	2.75	0.8661	0.8533	0.8417	0.8272	0.8019
10	78.08	26.15	12.4	6.04	2.52	0.8683	0.8551	0.8435	0.8285	0.8026
11	-	-	31.3	12.6	4.37	0.8858	0.8734	0.8622	0.8481	0.8241
12	-	37.83	16.81	7.89	3.21	0.9321	0.9187	0.9069	0.8923	0.8665
13	-	38.48	17.63	8.08	3.23	0.9407	0.9268	0.9144	0.8987	0.8726
15	-	24.8	12.91	6.86	3.08	0.8720	0.8596	0.8479	0.8337	0.8092
16	-	-	13.21	6.78	3.02	0.8985	0.8854	0.8739	0.8589	0.8335
18	75.77	24.13	11.44	5.76	2.49	0.9343	0.9212	0.9094	0.8949	0.8690
19	291.4	72.84	28.57	11.68	4.05	0.8789	0.8659	0.8548	0.8405	0.8158
22	53.62	19.13	9.358	4.8	2.0600	0.8210	0.8070	0.7954	0.7801	0.7552
23	52.07	18.7	9.444	4.9	2.1900	0.8251	0.8111	0.8000	0.7852	0.7597
25	30.81	12.81	7.04	3.9	1.8600	0.8152	0.8019	0.7905	0.7761	0.7507
26	24.68	10.65	6.07	3.51	1.7300	0.8225	0.8086	0.7965	0.7818	0.7566
27	36.7	14.86	7.963	4.37	2.0500	0.8176	0.8040	0.7924	0.7778	0.7528
51	-	15.73	8.447	4.57	2.1400	0.8172	0.8042	0.7925	0.7782	0.7531
52	61	20.75	10.63	5.54	2.47	0.8772	0.8638	0.8522	0.8378	0.8115
53	39.22	15.53	8.267	4.47	2.0800	0.8225	0.8096	0.7981	0.7837	0.7588
54	58.38	21.58	10.94	5.688	2.535	0.8726	0.8594	0.8474	0.8330	0.8074
55	-	19.72	9.678	4.92	2.14	0.8208	0.8077	0.7970	0.7816	0.7558
58	-	-	40.9	18.93	7.1350	0.8389	0.8268	0.8160	0.8024	0.7788
59	-	-	43.96	19.6	7.0130	0.8394	0.8273	0.8165	0.8029	0.7792
60	89.33	30.14	14.44	7.07	2.94	0.8501	0.8375	0.8261	0.8121	0.7875
61	282.2	76.36	31.22	13.22	4.61	0.9167	0.9037	0.8923	0.8780	0.8523
62	403.7	101.5	39.09	15.53	5.2	0.8824	0.8699	0.8585	0.8445	0.8203
63	-	18.03	9.548	5.09	2.3400	0.8205	0.8076	0.7961	0.7815	0.7567
64	53.74	20.23	10.26	5.4	2.42	0.8468	0.8331	0.8215	0.8075	0.7825
65	-	92.1	34.21	13.59	4.57	0.8757	0.8634	0.8520	0.8380	0.8137
67	48.44	18.12	9.243	4.86	2.17	0.8162	0.8031	0.7917	0.7777	0.7528
68	-	-	18.22	8.882	3.6	0.8670	0.8541	0.8426	0.8280	0.8032
69	131.3	43.21	19.85	9.421	3.76	0.8518	0.8392	0.8280	0.8139	0.7893
74	59.11	22.04	11.26	5.86	2.59	0.8448	0.8313	0.8196	0.8054	0.7804

75	-	26.22	13.16	6.83	3.03	0.8512	0.8385	0.8270	0.8132	0.7884
76	89.99	30.35	14.38	7.05	2.95	0.8515	0.8373	0.8268	0.8118	0.7872
77	86.21	29.4	14	6.88	2.86	0.8502	0.8369	0.8256	0.8115	0.7867
78	80.54	27.83	13.33	6.58	2.76	0.8501	0.8370	0.8256	0.8113	0.7865
79	-	-	11.38	6.04	2.71	0.8680	0.8549	0.8434	0.8284	0.8034
80	-	-	12.52	6.31	2.7	0.8682	0.8548	0.8432	0.8277	0.8017
81	-	24.62	12.04	6.09	2.62	0.8667	0.8537	0.8419	0.8274	0.8016
82	-	23.7	11.68	5.94	2.55	0.8665	0.8532	0.8424	0.8270	0.8013
87	37.7	14.84	7.9	4.34	2.02	0.8699	0.8560	0.8441	0.8296	0.8040
88	70.05	24.78	12.05	6.02	2.56	0.8461	0.8327	0.8216	0.8068	0.7820
89	462.2	74.24	25.5	10.12	3.63	1.0217	1.0076	0.9952	0.9801	0.9537
90	-	-	-	39.4	8.585	0.9163	0.9033	0.8920	0.8778	0.8526
91	95.47	32.17	15.17	7.37	3.02	0.8474	0.8347	0.8236	0.8098	0.7852
99	-	-	-	5.5	2.67	0.8669	0.8544	0.8430	0.8287	0.8041
100	-	-	-	7.16	3.22	0.8447	0.8322	0.8208	0.8067	0.7819
101	-	-	10.83	5.86	2.72	0.8682	0.8550	0.8432	0.8285	0.8029
102	-	27.87	14.23	7.4	3.26	0.8501	0.8371	0.8256	0.8118	0.7868
103	-	-	12.03	6.15	2.7	0.8678	0.8548	0.8432	0.8283	0.8030
104	-	29.01	14.01	7	2.98	0.8510	0.8382	0.8268	0.8124	0.7874
106	-	-	-	5.11	2.4800	0.8172	0.8042	0.7927	0.7783	0.7530
107	-	31.18	15.62	7.933	3.4100	0.8278	0.8153	0.8040	0.7902	0.7658
108	-	-	14.92	7.67	3.32	0.8735	0.8610	0.8494	0.8354	0.8102
109	-	-	9.176	5.17	2.4800	0.8204	0.8076	0.7962	0.7823	0.7564
110	45.85	17.95	9.401	4.98	2.25	0.8422	0.8292	0.8178	0.8029	0.7775
111	79.08	27.84	13.55	6.77	2.87	0.8710	0.8579	0.8469	0.8324	0.8065
112	115.6	38.59	18.04	8.728	3.58	0.9133	0.9000	0.8873	0.8728	0.8475
113	176.5	51.41	22.46	10.13	3.87	0.9020	0.8887	0.8774	0.8635	0.8379
115	2187	326.6	92.25	28.4	7.27	0.9249	0.9118	0.9001	0.8860	0.8608
116	215.6	55.82	22.23	9.526	3.525	0.9295	0.9163	0.9044	0.8897	0.8642
117	-	-	-	6.31	2.94	0.8422	0.8292	0.8178	0.8037	0.7784
118	-	-	15.74	8.114	3.484	-	-	0.8473	0.8333	0.8086
119	224.3	47.54	18.78	8.36	3.29	1.0304	1.0159	1.0029	0.9880	0.9611
120	-	-	2.168@239F	6.154	2.813	-	-	0.8203@239F	0.8568	0.8313
121	-	-	2318	275.2	27.68	1.0387	1.0257	1.0142	0.9998	0.9744
122	-	-	798.4	128.4	17.94	0.9484	0.9356	0.9242	0.9099	0.8858
124	-	-	-	24.03	6.573	0.9890	0.9762	0.9648	0.9505	0.9256
125	-	-	41.02	15.73	5.132	0.9137	0.9014	0.8902	0.8764	0.8522
126	176.8	44.72	18.57	8.438	3.309	0.9723	0.9589	0.9469	0.9322	0.9062
127	1249	213.4	65.73	22.19	6.194	0.9108	0.8976	0.8866	0.8722	0.8478
128	137.8	40.4	18.01	8.443	3.408	0.9336	0.9205	0.9089	0.8945	0.8693
129	405.6	94.58	35.7	14.34	4.778	0.9055	0.8932	0.8816	0.8677	0.8426
130	331.5	75.45	28.76	11.92	4.183	0.9360	0.9230	0.9116	0.8971	0.8721
131	-	-	229.9	56.89	12.03	1.0421	1.0296	1.0185	1.0046	0.9803
132	-	540.6	147.8	45.46	11.51	0.9427	0.9310	0.9202	0.9071	0.8839
133	-	36.24	17.91	8.879	3.7600	0.8292	0.8168	0.8056	0.7916	0.7675
134	-	42.42	20.68	10.11	4.2650	0.8313	0.8189	0.8077	0.7938	0.7696

135	-	9.130@158F	6.337@185F	12.15	4.686	0.8657	0.8532	0.8420	0.8281	0.8036
136	-	63.22	28.16	12.89	4.886	0.8529	0.8406	0.8296	0.8158	0.7918
137	-	11.78@157F	8.054@185F	15.85	5.891	0.8659	0.8534	0.8183@185F	0.8283	0.8039
138	-	-	37.07	16.52	6.047	0.8542	0.8420	0.8312	0.8177	0.7940
139	668.6	125.5	41.19	14.76	4.494	0.8823	0.8698	0.8584	0.8449	0.8203
140	-	10.64@176F	8.00@194F	-	5.961	-	-	-	-	0.9292
141	-	108	39.14	15.45	5.119	0.9189	0.9066	0.8952	0.8812	0.8571
142	-	-	42.52	16.6	5.468	-	-	0.9474	0.9328	0.9077
143	-	77.75	32.9	14.4	5.233	-	0.9016	0.8905	0.8767	0.8526
144	-	-	4.527@239F	18.39	6.395	-	-	0.9149@239F	0.9509	0.9260
145	-	-	5.748@239F	2.971@275F	8.444	-	-	0.8614@239F	0.8486@275F	0.8718
146	-	3.609@239F	2.571@275F	13.93	4.907	-	0.9118@239F	0.8988@275F	0.9469	0.9218
152	-	-	10.21	5.671	2.677	0.8659	0.8530	0.8414	0.8271	0.8020
153	-	-	13.6	7.19	3.191	0.8458	0.8331	0.8217	0.8076	0.7827
155	-	-	43.83@176F	27.48@194F	19.09	0.9598	0.9482	0.9133@176F	0.9076@194F	0.9024
156	-	-	2.668@239F	8.924	3.58	-	-	0.8023@239F	0.8372	0.8125
157	-	29.28	14.49	7.435	3.268	-	0.8344	0.8232	0.8094	0.7856
158	-	-	2.183@239F	6.549	2.887	-	-	0.7966@239F	0.8328	0.8079
159	-	24.66	12.64	6.63	2.963	-	0.8325	0.8212	0.8074	0.7829
161	86.55	29.07	13.7	6.656	2.717	0.8664	0.8530	0.8413	0.8268	0.8009
162	95.74	31.15	14.44	6.918	2.809	0.8483	0.8355	0.8241	0.8099	0.7849
163	23.64	10.24	5.73	3.258	1.5840	0.8104	0.7976	0.7858	0.7712	0.7455
164	-	-	16.86	8.526	3.5950	0.8270	0.8146	0.8037	0.7897	0.7654
165	-	-	346.5	70.72	12.16	0.9926	0.9796	0.9682	0.9538	0.9287
166	-	-	290.6	60.38	10.93	0.9522	0.9395	0.9282	0.9140	0.8893
167	110.8	35.08	16.23	7.778	3.112	0.8745	0.8614	0.8495	0.8350	0.8093
168	-	49.87	21.48	9.555	3.555	0.8705	0.8574	0.8456	0.8312	0.8055
169	164.8	48.12	20.77	9.332	3.48	0.8518	0.8390	0.8279	0.8139	0.7892
170	303.3	63.76	24.96	10.68	3.95	1.0059	0.9922	0.9802	0.9654	0.9392
171	-	91.61	31.97	12.65	4.317	0.9960	0.9826	0.9707	0.9560	0.9302
172	-	-	110.9	33.75	8.371	0.9081	0.8957	0.8847	0.8712	0.8472
173	392.4	100.7	39.42	15.94	5.21	0.9008	0.8879	0.8765	0.8623	0.8373
174	-	-	17.56	8.384	2.882	0.9275	0.9145	0.9029	0.8885	0.8631
175	-	36.13	17.25	8.538	3.536	0.8806	0.8681	0.8568	0.8429	0.8184
176	-	-	4.908@158F	3.659@185F	2.8790	0.8196	0.8068	0.7748@158F	0.7651@185F	0.7565
177	592.3	132.2	47.79	18.16	5.583	0.9075	0.8946	0.8832	0.8692	0.8446
178	109.3	34.68	15.92	7.546	2.993	0.8705	0.8577	0.8461	0.8320	0.8069
179	-	7830	837.2	133.7	18.28	1.0372	1.0240	1.0122	0.9977	0.9722
180	67.99	24.34	11.95	6.13	2.633	0.8388	0.8260	0.8146	0.8007	0.7759
181	253.3	69.09	28.47	12.16	4.261	0.8928	0.8798	0.8684	0.8540	0.8290
182	2514	369.8	104.1	32.4	8.2630	0.8325	0.8204	0.8096	0.7961	0.7725

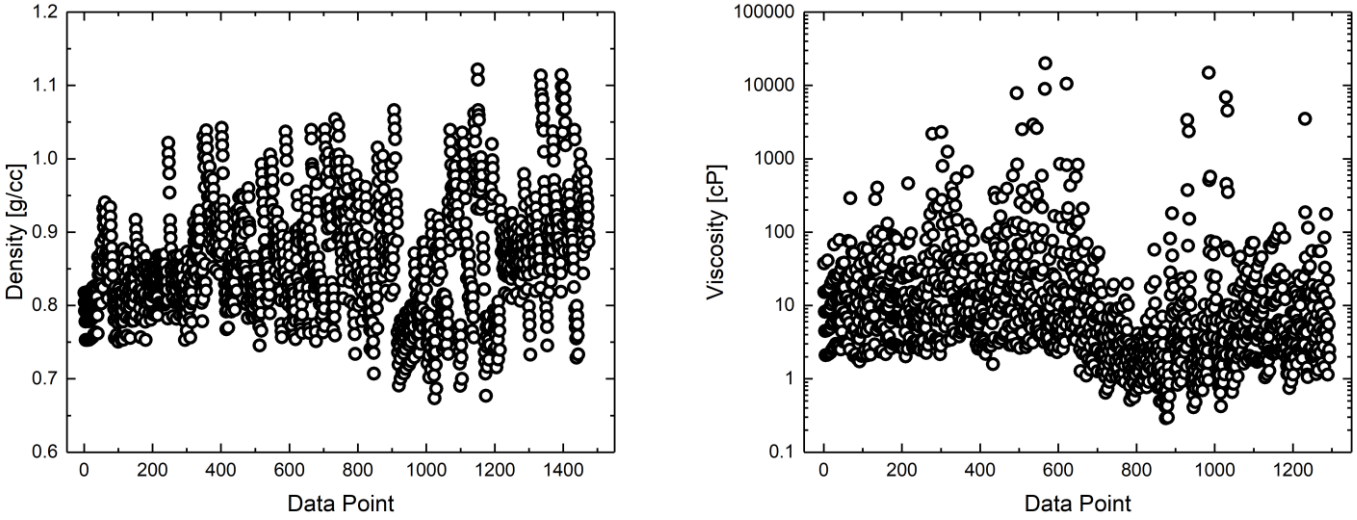
183	121.2	33.24	14.5	6.755	2.6920	0.8214	0.8088	0.7975	0.7835	0.7589
184	217.6	49.77	19.48	8.27	3.0140	0.8168	0.8043	0.7929	0.7789	0.7541
188	-	-	16.96	8.31	3.433	0.9019	0.8889	0.8773	0.8628	0.8376
189	-	-	10.36@158F	6.936@185F	5.073	0.9497	0.9369	0.9050@158F	0.8955@185F	0.8865
190	-	-	7.031@177.4F	5.689@196F	4.9040	0.8296	0.8171	0.7795@176F	0.7733@194F	0.7677
191	-	27.57	14.05	7.248	3.1240	0.8252	0.8125	0.8012	0.7873	0.7626
192	2931	406.7	112.1	34.13	8.429	0.9106	0.8982	0.8872	0.8734	0.8494
193	-	61.64	27.52	12.68	4.83	0.9076	0.8954	0.8842	0.8704	0.8463
196	2616	327	88.02	27.23	7.083	0.9554	0.9432	0.9323	0.9187	0.8951
197	-	-	5.456@176F	4.493@194F	3.8240	0.8243	0.8119	0.7744@176F	0.7681@194F	0.7626
199	236.1	62.68	25.85	11.47	4.087	0.9025	0.8900	0.8789	0.8650	0.8408
200	-	-	586.9@176F	217.1@194F	106.1	1.0393	1.0277	0.9927@176F	0.9869@194F	0.9817
202	-	30.69	14.86	7.457	3.162	0.8774	0.8650	0.8538	0.8398	0.8155
203	-	-	-	20000000	8970	-	-	-	-	-
204	-	-	-	-	20000	-	-	-	-	-
205	-	-	5.433@239F	3.910@275F	7.4790	0.8377	0.8249	0.7642@239F	0.7514@275F	0.7745
206	-	-	3.296@239F	11.83	4.479	-	-	0.9285@239F	0.9658	0.9395
207	-	-	5.278@239F	3.595@275F	7.733	-	-	0.8390@239F	0.8265@275F	0.8494
208	42.83	17.75	9.631	5.317	2.496	0.8657	0.8526	0.8411	0.8267	0.8018
209	-	-	12.26	6.478	2.863	-	0.8317	0.8202	0.8061	0.7816
210	76.13	26.68	15.75	6.347	2.6290	0.8261	0.8133	0.8018	0.7878	0.7631
211	165.1	53.75	24.5	11.35	4.2210	0.8327	0.8205	0.8095	0.7957	0.7721
215	-	-	5.026	3.394	7.313	1.0400	1.0271	1.0154	1.0011	0.9759
216	-	3.886@239F	2.711@275F	16.56	5.512	0.9414	0.9294	0.9187	0.9050	0.8817
218	-	-	6.418@239F	4.114@275F	10.13	1.0080	0.9947	0.9827	0.9677	0.9418
219	851.8	157.1	52.7	18.89	5.864	0.9444	0.9320	0.9210	0.9070	0.8834
220	-	-	3.470@239F	2.569@275F	4.5940	0.8314	0.8183	0.8067	0.7922	0.7669
223	117.5	36.36	16.68	7.837	3.2040	0.8221	0.8092	0.7979	0.7837	0.7592
224	-	-	9.052@239F	5.406@275F	15.05	-	1.0542	0.9946@239F	0.9818@275F	1.0045
225	10500	815.9	170.7	41.98	9.121	0.9525	0.9398	0.9285	0.9150	0.8916
226	6.673@239F	4.253@275F	212.6	50.16	10.46	0.9958@239F	0.9833@275F	1.0458	1.0310	1.0059
228	5.272@239F	434.1	110.3	31.72	7.941	0.8810@239F	0.9387	0.9278	0.9140	0.8906
229	-	29.46	15.15	7.923	3.456	0.8722	0.8596	0.8482	0.8341	0.8096
230	4.992@239F	3.395@275F	74.56	25.25	7.256	0.9184@239F	0.9053@275F	0.9700	0.9547	0.9291
231	564.1	127.8	48.29	18.75	6.178	0.9291	0.9158	0.9046	0.8903	0.8662
232	-	-	831.8	140.4	19.9	0.9962	0.9837	0.9726	0.9587	0.9345
235	20.19	7.981	4.423	2.521	1.274	0.8731	0.8594	0.8473	0.8320	0.8055

236	3.105@239F	2.209@275F	33.25	12.79	4.316	0.884@239F	0.8754@275F	0.9393	0.9244	0.8989
237	209.9	55.38	22.99	9.921	3.732	0.9031	0.8905	0.8790	0.8650	0.8409
500	12.47	5.854	3.515	2.125	1.1080	0.8012	0.7878	0.7756	0.7606	0.7340
501	70.32	18.97	8.569	4.217	1.84	0.9774	0.9628	0.9497	0.9333	0.9046
502	22.63	9.155	4.966	2.771	1	0.8679	0.8541	0.8417	0.8262	0.7994
503	-	16.73	7.956	4.023	1.788	0.9647	0.9498	0.9375	0.9215	0.8939
504	30.41	11.6	6.058	3.274	1.523	0.8450	0.8317	0.8196	0.8048	0.7786
505	-	44.29	16.72	6.988	2.559	0.8962	0.8829	0.8714	0.8569	0.8315
506	17.16	7.428	4.225	2.486	1.266	0.8848	0.8705	0.8578	0.8420	0.8140
507	-	-	-	48.48	7.307	0.9615	0.9474	0.9350	0.9197	0.8927
509	52.8	19.09	9.534	4.884	2.142	0.8469	0.8337	0.8220	0.8076	0.7828
510	-	6.552	3.86	2.328	1.2360	0.8063	0.7932	0.7815	0.7665	0.7407
511	14.92	6.832	4.008	2.392	1.2430	0.8043	0.7909	0.7789	0.7640	0.7377
512	3.612	2.184	1.517	1.065	0.6449	0.7772	0.7634	0.7510	0.7352	0.7072
513	4.653	2.64	1.794	1.219	0.7328	0.8711	0.8571	0.8440	0.8277	0.7988
514	6.749	3.677	2.407	1.591	0.9086	0.8373	0.8235	0.8110	0.7956	0.7684
516	8.983	4.484	2.844	1.84	1.075	1.0152	0.9998	0.9860	0.9690	0.9387
517	15.98	6.87	3.928	2.358	1.24	0.9498	0.9356	0.9231	0.9071	0.8790
518	19.33	8.494	4.896	2.896	1.476	0.9069	0.8932	0.8808	0.8658	0.8389
519	-	-	-	1.808	1.06	1.0042	0.9890	0.9752	0.9583	0.9289
520	-	7.951	4.62	2.725	1.422	0.8880	0.8740	0.8616	0.8466	0.8200
521	9.125	4.709	2.935	1.89	1.104	0.9409	0.9262	0.9133	0.8974	0.8693
522	6.24	3.606	2.388	1.671	0.9911	0.9321	0.9175	0.9043	0.8889	0.8607
523	9.609	4.977	3.222	2.109	1.193	0.8810	0.8675	0.8556	0.8407	0.8136
524	-	-	2.201	1.51	0.9151	-	-	0.9929	0.9756	0.9453
525	11.71	5.685	3.515	2.187	1.81	0.8907	0.8768	0.8644	0.8488	0.8216
526	-	-	-	19.72	4.616	1.0662	1.0530	1.0412	1.0266	1.0007
527	-	-	-	10.22	3.301	0.9508	0.9383	0.9268	0.9124	0.8877
528	2.265	1.492	1.102	0.8026	0.5156	0.7636	0.7487	0.7360	0.7194	0.6907
529	2.948	1.864	1.345	0.9594	0.6010	0.7704	0.7563	0.7436	0.7279	0.7004
530	2.551	1.663	1.218	0.8776	0.5597	0.7798	0.7656	0.7528	0.7366	0.7081
531	-	2.323	1.627	1.137	0.6940	0.7771	0.7629	0.7505	0.7347	0.7071
532	-	2.842	1.953	1.335	0.7960	0.7826	0.7685	0.7562	0.7408	0.7135
533	4.16	2.519	1.762	1.224	0.7454	0.7898	0.7757	0.7633	0.7478	0.7209
534	-	3.453	2.331	1.559	0.9054	0.7874	0.7737	0.7612	0.7460	0.7190
535	-	-	2.742	1.795	1.0240	0.7916	0.7780	0.7658	0.7506	0.7240
536	-	3.729	2.496	1.67	0.9647	0.7999	0.7861	0.7737	0.7585	0.7314
537	-	-	3.209	2.062	1.1500	0.7964	0.7828	0.7708	0.7558	0.7292
538	4.288	2.575	1.802	1.254	0.7648	0.8712	0.8565	0.8442	0.8275	0.7988
539	6.311	3.515	2.351	1.576	0.9119	0.8282	0.8139	0.8017	0.7864	0.7590
540	-	-	4.29	2.664	1.4240	0.8021	0.7888	0.7729	0.7621	0.7361
541	-	-	-	4.191	2.0830	0.8118	0.7988	0.7873	0.7728	0.7475
542	17.62	7.752	4.432	2.589	1.302	0.8361	0.8228	0.8107	0.7958	0.7693
543	2.83	1.853	1.346	0.9569	-	0.8863	0.8695	0.8543	0.8353	-
544	57.78	21	10.66	5.589	2.49	0.8853	0.8725	0.8611	0.8469	0.8220
545	6.029	3.178	2.052	1.335	0.7598	0.7898	0.7761	0.7635	0.7482	0.7210
546	2.768	1.64	1.146	0.801	0.4940	0.7751	0.7606	0.7478	0.7315	0.7020

547	2.302	1.456	1.055	0.762	0.4820	0.7865	0.7718	0.7588	0.7424	0.7128
548	7.054	4.273	2.976	2.05	1.223	0.9229	0.9097	0.8979	0.8833	0.8576
549	0.9413	0.6822	0.5412	0.4184	0.2900	0.7507	0.7354	0.7219	0.7048	0.6734
550	0.9274	0.6842	0.5455	0.4268	0.2982	0.7662	0.7505	0.7365	0.7189	0.6866
551	1.985	1.434	1.12	0.8566	0.5775	0.8793	0.8646	0.8514	0.8349	0.8052
552	81.99	28.25	13.91	6.976	2.936	0.9185	0.9053	0.8935	0.8789	0.8532
553	180.3	48.27	20.19	8.935	3.345	0.9090	0.8950	0.8841	0.8696	0.8440
554	17.52	7.846	4.516	2.642	1.3220	0.8059	0.7926	0.7808	0.7662	0.7401
555	5.259	3.045	2.081	1.413	0.8280	0.8152	0.8013	0.7886	0.7727	0.7443
556	8.434	4.584	2.985	1.938	1.0750	0.8136	0.8004	0.7886	0.7738	0.7470
557	9.689	4.524	2.742	1.697	0.9176	0.8050	0.7879	0.7758	0.7608	0.7338
559	-	23.18	11.11	5.595	2.423	0.9412	0.9279	0.9159	0.9010	0.8750
560	20.22	7.36	4.012	2.325	1.1920	1.0394	1.0235	1.0093	0.9916	0.9607
561	12.3	6.559	4.218	2.706	1.482	0.9624	0.9489	0.9367	0.9216	0.8949
562	-	3387	374.8	65.38	11.21	0.9785	0.9661	0.9550	0.9412	0.9171
563	-	-	2366	152.4	15.32	0.9891	0.9765	0.9654	0.9513	0.9269
564	24.53	10.11	5.628	3.25	1.635	0.9500	0.9366	0.9247	0.9099	0.8838
565	1.507	1.054	0.8085	0.6118	0.4080	0.7653	0.7505	0.7372	0.7205	0.6903
566	1.976	1.329	0.9989	0.7389	0.4810	0.7730	0.7586	0.7455	0.7292	0.7000
567	6.132	3.351	2.226	1.494	0.8817	1.0357	1.0211	1.0079	0.9914	0.9624
568	-	-	1.72	1.197	0.738	1.0215	1.0063	0.9927	0.9758	0.9461
569	5.558	3.349	2.31	1.569	0.9162	0.9119	0.8968	0.8834	0.8665	0.8369
570	3.214	2.109	1.546	1.114	0.696	0.8845	0.8698	0.8565	0.8399	0.8106
571	6.847	3.81	2.535	1.694	0.987	0.8693	0.8554	0.8430	0.8275	0.8001
572	10.25	5.331	3.386	2.16	1.188	0.8319	0.8186	0.8067	0.7918	0.7655
573	6.203	3.59	2.434	1.641	0.9606	0.8246	0.8109	0.7986	0.7834	0.7563
574	-	14900	512.7	54.28	8.15	1.0620	1.0492	1.0378	1.0236	0.9987
575	571.9	75.06	25.51	10.38	3.792	0.9927	0.9803	0.9692	0.9557	0.9320
576	-	-	6.162@176F	4.684@194F	3.776	1.1217	1.1078	1.0662@176F	1.0593@194F	1.0531
577	49.76	17.81	9.31	5.086	2.379	0.9950	0.9822	0.9706	0.9563	0.9313
578	72.45	24.4	12.11	6.278	2.772	1.0019	0.9890	0.9775	0.9634	0.9386
580	3.558	2.334	1.706	1.231	0.7823	0.8924	0.8782	0.8657	0.8497	0.8218
581	1.638	1.124	0.8513	0.6377	0.4210	0.7513	0.7367	0.7235	0.7070	0.6769
582	6.109	3.437	2.308	1.541	0.8949	0.7845	0.7707	0.7586	0.7434	0.7162
583	-	5.061	3.235	2.075	1.1480	-	0.7795	0.7675	0.7527	0.7262
584	-	-	7.454	4.308	2.1260	-	-	0.7858	0.7713	0.7460
586	-	6918	454.8	62.54	10.08	0.9833	0.9709	0.9596	0.9455	0.9213
587	-	4512	351	56.13	10.13	1.0200	0.9981	0.9873	0.9738	0.9503
588	-	8.302	5.023	3.051	1.5890	-	0.7934	0.7815	0.7668	0.7412
589	3.348	2.097	1.502	1.064	0.6590	0.7861	0.7720	0.7594	0.7435	0.7155
590	-	3.082	2.109	1.436	0.8515	0.7953	0.7813	0.7691	0.7537	0.7265
591	16.49	7.89	4.788	2.836	1.4800	0.8053	0.7921	0.7801	0.7654	0.7394
592	9.55	4.793	3.042	1.937	1.084	0.9436	0.9294	0.9168	0.9011	0.8730
593	40.78	15.76	8.394	4.598	2.163	0.9158	0.9025	0.8908	0.8761	0.8502
594	46.14	18.04	9.57	5.147	2.359	0.8811	0.8679	0.8563	0.8420	0.8167
595	20.896	9.192	5.34	3.13	1.609	0.9077	0.8941	0.8820	0.8667	0.8402
596	32.166	13.572	7.486	4.243	2.038	0.8795	0.8650	0.8540	0.8393	0.8136

597	24.186	10.599	6.044	3.529	1.779	0.9104	0.8967	0.8846	0.8695	0.8426
598	29.403	12.746	7.113	4.052	2.055	0.8676	0.8631	0.8510	0.8361	0.8100
599	56.83	18.48	8.71	4.34	1.86	0.9261	0.9103	0.8997	0.8844	0.8574
600	71.383	20.843	9.276	4.396	1.81	0.9108	0.8967	0.8843	0.8690	0.8418
601	70.973	21.151	9.459	4.551	1.928	0.8817	0.8683	0.8566	0.8418	0.8157
602	25.825	10.81	6.033	3.379	1.697	0.9057	0.8918	0.8794	0.8642	0.8373
603	33.5	13.32	7.164	3.93	1.841	0.8723	0.8588	0.8470	0.8323	0.8063
604	41.07	15.365	7.917	4.186	1.884	0.9150	0.9011	0.8888	0.8736	0.8466
605	45.7	15.77	7.784	4.014	1.776	0.8829	0.8694	0.8574	0.8425	0.8165
606	9.459	4.66	2.932	1.861	1.045	0.9794	0.9651	0.9521	0.9363	0.9083
607	11.01	5.444	3.4	2.122	1.15	0.8899	0.8760	0.8639	0.8487	0.8219
608	-	4.073	2.678	1.763	-	-	0.8865	0.8739	0.8581	0.8421
609	-	-	3.708	2.36	1.2810	0.7989	0.7857	0.7737	0.7590	0.7328
610	65.32	22.03	10.54	5.257	2.227	0.9424	0.9284	0.9164	0.9014	0.8748
611	61.43	20.81	10.08	5.017	2.158	0.9173	0.9039	0.8916	0.8766	0.8500
612	74.55	24.03	11.24	5.491	2.283	0.8843	0.8713	0.8595	0.8451	0.8196
613	81.31	24.89	11.49	5.506	2.271	0.9470	0.9330	0.9209	0.9058	0.8796
614	92.05	29.21	13.3	6.287	2.5	0.9222	0.9086	0.8967	0.8818	0.8555
615	111.17	30.76	13.17	5.977	2.346	0.8888	0.8755	0.8639	0.8494	0.8239
616	-	-	3.542@239F	2.431@275F	5.154	1.1134	1.0998	1.0877	1.0727	1.0461
617	-	3.119@239F	2.151@275F	17.24	4.473	1.0808	1.0684	1.0550	1.0384	1.0094
618	84.82	25.56	12.1	6.123	2.659	0.9684	0.9553	0.9438	0.9296	0.9046
619	-	1.501@239F	1.165@275F	3.759	1.9260	0.8098	0.7968	0.7852	0.7707	0.7454
620	3.322	2.208	1.619	1.165	0.749	0.8934	0.8782	0.8646	0.8475	0.8177
622	5.079	3.144	2.212	1.534	0.9186	0.9031	0.8889	0.8763	0.8606	0.8329
623	8.001	4.507	3.009	1.992	1.138	0.9170	0.9031	0.8909	0.8757	0.8489
625	-	17.34	8.227	4.26	1.945	1.0373	1.0241	1.0123	0.9973	0.9709
626	15.51	7.591	4.729	2.872	1.582	0.9582	0.9448	0.9336	0.9187	0.8931
627	-	-	13.46	6.189	2.488	0.9488	0.9352	0.9231	0.9079	0.8815
628	-	25.42	11.64	5.593	2.333	0.9169	0.9035	0.8916	0.8770	0.8514
629	-	20.78	10.07	5.08	2.213	0.8825	0.8697	0.8582	0.8439	0.8186
631	-	-	2.741@239F	1.903@275F	4.004	1.1141	1.0984	1.0845	1.0668	1.0359
632	-	-	2.859@239F	14.22	4.128	-	-	0.8742@239F	0.9103	0.8853
633	-	-	2.932@239F	24.19	4.612	1.0972	1.0814	1.0672	1.0496	1.0185
634	3503.2	186.8	45.1	14.17	4.323	0.9533	0.9404	0.9290	0.9146	0.8894
637	-	-	1.140@239F	1.059@275F	1.419	0.9450	0.9308	0.9182	0.9024	0.8748
638	114.8	31.42	13.71	6.303	2.58	0.9639	0.9507	0.9389	0.9243	0.8991
639	2.022@239F	34.36	14.68	6.701	2.688	0.8593@239F	0.9217	0.9098	0.8951	0.8695
640	55.23	19.03	9.496	4.881	2.184	0.8884	0.8755	0.8641	0.8499	0.8250
641	-	-	-	3.299@239F	2.296@275F	-	-	-	1.0395@239F	1.0261@275F
642	13.59	6.207	3.686	2.218	1.1630	0.7956	0.7821	0.7703	0.7551	0.7289
643	17.1	7.525	4.369	2.567	1.3180	0.7996	0.7861	0.7742	0.7591	0.7333

645	54.77	18.37	9.324	4.934	2.277	0.9729	0.9594	0.9474	0.9325	0.9070
646	54.88	14.76	6.913	3.533	1.632	1.0065	0.9923	0.9798	0.9639	0.9363
647	16.6	7.634	4.57	2.752	1.446	0.9108	0.8973	0.8854	0.8701	0.8439
648	-	84.24	32.91	13.21	4.517	0.9447	0.9316	0.9200	0.9053	0.8800
652	176.2	6.57	3.688	2.16	1.143	0.9827	0.9683	0.9554	0.9392	0.9114
654	1.937@239F	22.26	10.86	5.554	2.5	0.8869@239F	0.9455	0.9346	0.9206	0.8967



(a) (b)

Figure S1: Experimental (a) density and (b) dynamic viscosity of all 305 hydrocarbon molecules from API Project 42 [1].

Models with Combined Static and Dynamic Descriptors

The best 2 and 3 static and dynamic descriptors are Equations (S1) and (S2). Model I is a function of the simulation-calculated density (rho) and Ghose-Crippen LogKow ($ALogP$) [2]. Model III is a function of rho, $ALogP$, and pairwise interaction energy ($epair$). $epair$ quantify strength of inter and intra-molecular interactions.

Model I: $$\rho(T) = f(ALogP, rho) \quad \text{(S1)}$$

Model II: $$\rho(T) = f(ALogP, rho, epair) \quad \text{(S2)}$$

The best 2, 3, and 4 static and dynamic descriptors are Equations (S3), (S4), and (S5). Model I is a function of complexity of a system ($fragC$), bonding energy ($ebond$) of the molecule. Model III is a function of kinetic energy, number of rotatable bonds ($nRotB$) in the molecule, and lipophilicity index ($XLogP$). Model III is a function of temperature (T), fraction of rotatable bond ($RotBFrac$), excluding terminal bonds in a molecule, and Crippen's molar refractivity ($CrippenMR$), and sphericity (b) of molecules. b quantify how spherical a molecule is. If b is 0 then a molecule is perfectly spherical in shape. A higher b mean a molecule is further away from the spherical shape or distribution of its atoms. $ALogP$ and $XLogP$ are the lipophilicity indexes which were calculated using different approaches. Lipophilicity indexes quantify the interaction between molecules of a system.

Model I: $$\log\eta(T) = f(fragC, ebond) \quad \text{(S3)}$$

Model II: $$\log\eta(T) = f(ke, nRotB, XLogP) \quad \text{(S4)}$$

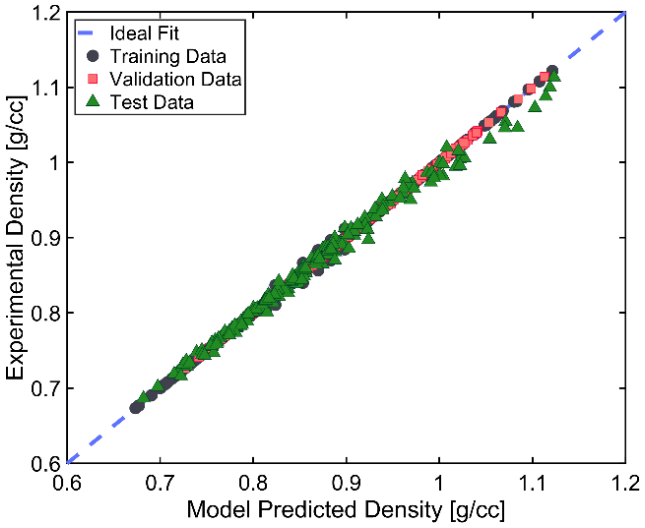
Model III: $$\log\eta(T) = f(T, RotBFrac, CrippenMR, b) \quad \text{(S5)}$$

Table S3 lists the R^2 and RMSE values for the density and viscosity models with combined static and dynamic descriptors for the training, validation, and test data sets. The average R^2 value of the training, validation, and test data sets is also listed for the comparison between the models. The maximum value of VIF out of VIFs for each predictor is also listed to indicate the degree of multicollinearity.

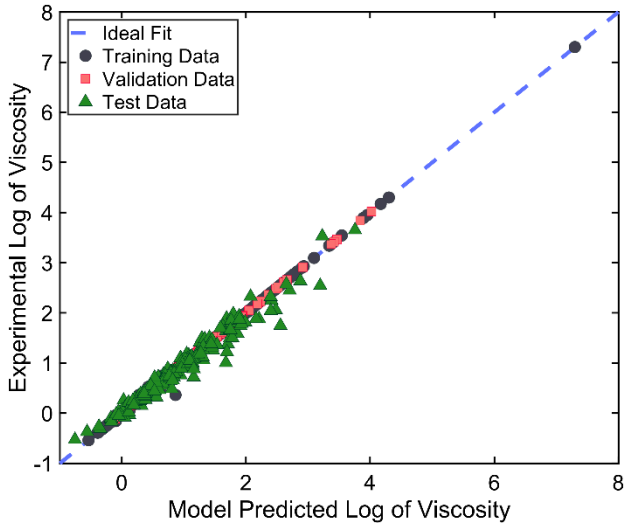
Table S3: Model assessment parameters for the density and viscosity models with combined static and dynamic descriptors.

Parameter		Density Models		Viscosity Models		
		Model I	Model II	Model I	Model II	Model III
Training	R^2	0.999	1.000	0.998	0.992	1.000
	RMSE	0.003	0.001	0.028	0.066	0.009
Validation	R^2	0.999	1.000	1.000	0.992	1.000
	RMSE	0.003	0.000	0.012	0.065	0.000
Test	R^2	0.982	0.990	0.818	0.947	0.947
	RMSE	0.011	0.008	0.288	0.155	0.156
Average R^2		0.993	0.997	0.939	0.977	0.982
Maximum VIF		0.999	1.000	1.109	4.094	2.407

Figures S2(a) and S2(b) show density and viscosity predicted using their best models of combined static and dynamic descriptors for all data sets over a wide temperature range. The blue dashed line represents an ideal prediction. The model-predicted density for the training, validation, and test data sets is shown as black circles, red squares, and green triangle, respectively.



(a)



(b)

Figure S2: Model predicted (a) density (Equation S2) and (b) viscosity (Equation S5) by the models with combined static and dynamic descriptors for the training (black circle), validation (red square), and test data (green triangle) sets. The blue dash lines represent the ideal prediction.

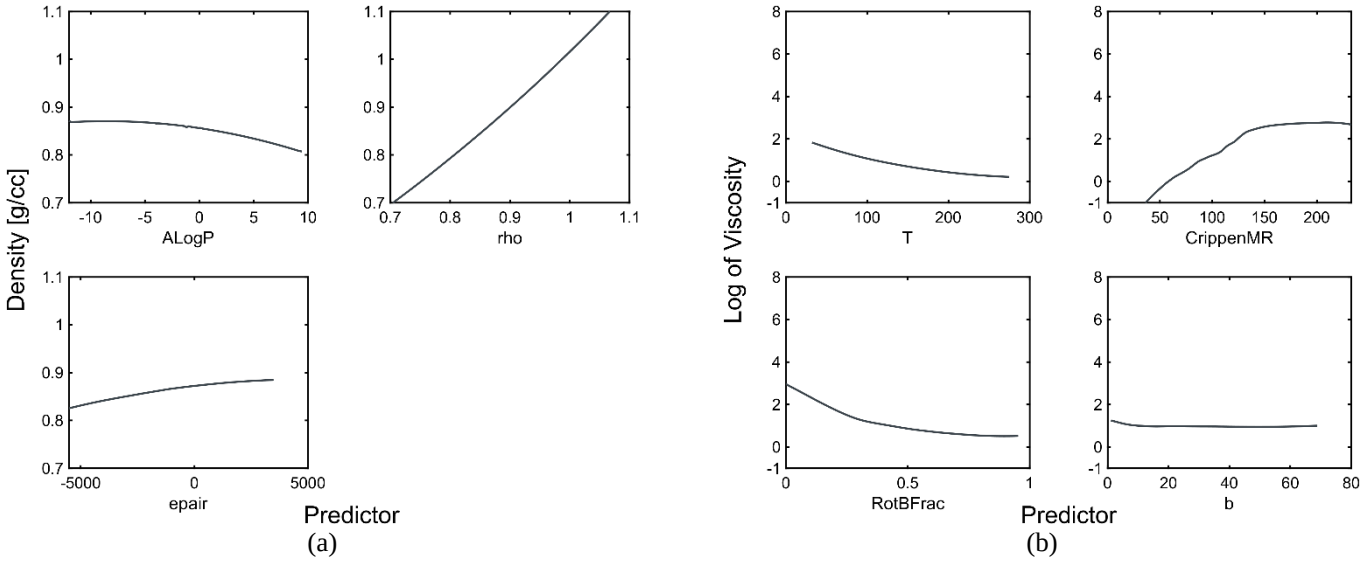


Figure S3: Partial dependency plots of predictors in the best (a) density model (Equation S2) and (b) viscosity model (Equation S5) with combined static and dynamic descriptors.

Density Models with Dynamic Descriptors excluding Simulation-Calculated Density

The best three models with 1, 2, and 3 dynamic descriptors excluding simulation-calculated density (rho) for predicting the temperature-dependent density of the hydrocarbons are Equations (S6), (S7), and (S8). Model I is only a function of van der Waals energy long-range tail correction ($etail$). Models II is a function of $etail$ and energy due to improper interaction ($eimp$, higher for more rigidity molecule). Model III has an additional term which is the length of the molecule (L_y). It was noted that length of the molecules in any direction (L_x, L_y, L_z) resulted in similar predicting performance when used in Equation (S8), likely because the dynamic descriptors were calculated from equilibration MD simulations with a cubic simulation box.

Model I $$\rho(T) = f(etail) \quad \text{(S6)}$$

Model II $$\rho(T) = f(etail, eimp) \quad \text{(S7)}$$

Model III $$\rho(T) = f\left(etail, eimp, L_y\right) \quad \text{(S8)}$$

Table S4 lists the R^2 and RMSE values for the density models with dynamic descriptors excluding simulation-calculated density for the training, validation, and test data sets. The average R^2 value of the training, validation, and test data sets is also listed for the comparison between the models. The maximum value of VIF out of VIFs for each predictor is also listed to indicate the degree of multicollinearity.

Table S4: Model assessment parameters for the density models with dynamic descriptors excluding simulation-calculated density.

Parameter		Model I	Model II	Model III
Training	R^2	0.928	0.979	1.000
	RMSE	0.020	0.011	0.001
Validation	R^2	0.913	0.989	1.000
	RMSE	0.024	0.008	0.000
Test	R^2	0.929	0.970	0.973

	RMSE	0.022	0.014	0.013
Average R^2		0.923	0.980	0.991
Maximum VIF		1.000	3.246	3.336

Figures S4(a) shows density predicted using the best models of dynamic descriptors excluding simulation-calculated density for all data sets over a wide temperature range. The blue dashed line represents an ideal prediction. The model-predicted density for the training, validation, and test data sets is shown as black circles, red squares, and green triangle, respectively. Figures S4(b) shows partial dependency plots of predictors in the best density model predicted of dynamic descriptors excluding simulation-calculated density

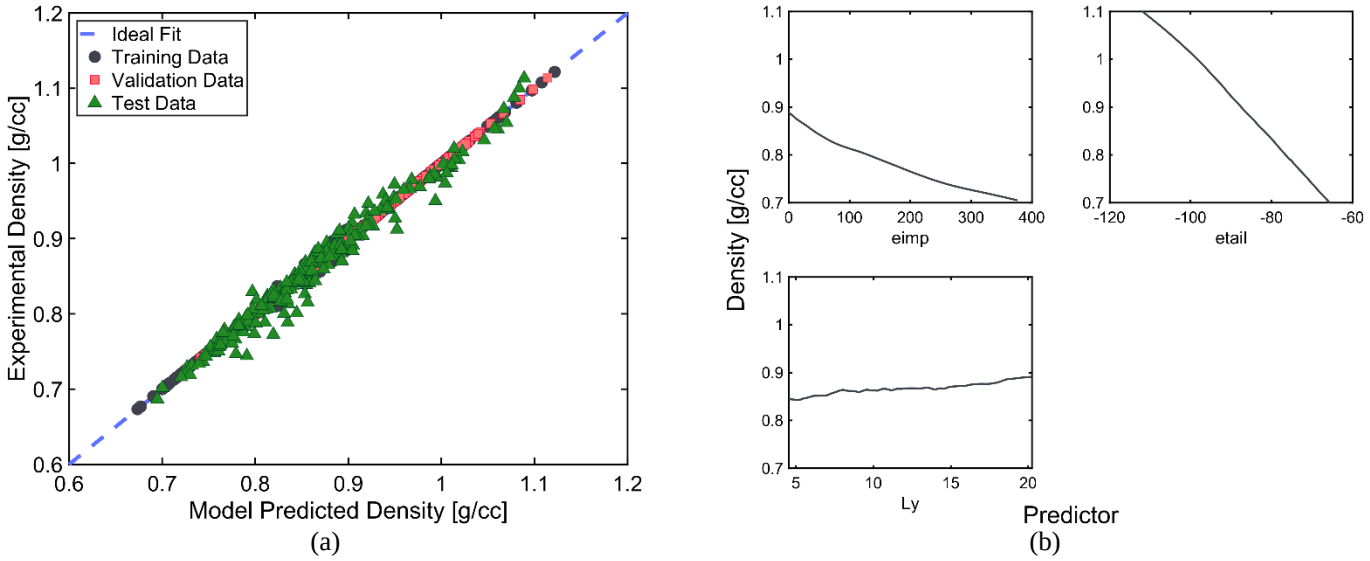


Figure S4: (a) Model predicted density (Equation S8) by the models with dynamic descriptors for the training (black circle), validation (red square), and test data (green triangle) sets. The blue dash lines represent the ideal prediction. (b) Partial dependency plots of predictors in the best density model (Equation S8) with dynamic descriptors.

Additional Supplementary Materials

The following supplementary materials are provided in supplementary.zip which include:

- Schematic of all the molecules
- Definition of important molecular descriptors.
- All experimental data with the important static and dynamic descriptors of all the molecules
- LAMMPS data files of all the molecules and input files to run the MD simulations
- MATLAB files of the best models to predict temperature dependent density and viscosity.

References

[1] American Petroleum Institute, 1967, *Properties of Hydrocarbons of High Molecular Weight Synthesized by Research Project 42 of the American Petroleum Institute*, New York.

[2] Todeschini, R., and Consonni, V., 2010, *Molecular Descriptors for Chemoinformatics*.