Decane; Scaffold number: 1; Isomeric number: 1; SMILES: CCCCCCCC

2-Methylnonane; Scaffold number: 2; Isomeric number: 2; SMILES: CC(C)CCCCCC

3-Methylnonane; Scaffold number: 3; Isomeric number: 3_1; SMILES: C[C@H](CC)CCCCC

3-Methylnonane; Scaffold number: 4; Isomeric number: 3_2; SMILES: C[C@@H](CC)CCCCC

4-Methylnonane; Scaffold number: 5; Isomeric number: 4_1; SMILES: C[C@H](CCC)CCCC

4-Methylnonane; Scaffold number: 6; Isomeric number: 4_2; SMILES: C[C@@H](CCC)CCCC

5-Methylnonane; Scaffold number: 7; Isomeric number: 5; SMILES: CC(CCC)CCCC

2,2-Dimethyloctane; Scaffold number: 8; Isomeric number: 6; SMILES: CC(C)(CCCCC)C

2,3-Dimethyloctane; Scaffold number: 9; Isomeric number: 7_1; SMILES: CC(C)[C@H](CCCCC)C

2,3-Dimethyloctane; Scaffold number: 10; Isomeric number: 7_2; SMILES: CC(C)[C@@H](CCCCC)C

2,4-Dimethyloctane; Scaffold number: 11; Isomeric number: 8_1; SMILES: CC(C)C[C@H](CCCC)C

$$\mathsf{H}_3\mathsf{C} \underbrace{\hspace{1cm} \mathsf{CH}_3}_{\mathsf{H} \;\; \mathsf{CH}_3} \; \mathsf{CH}_3$$

2,4-Dimethyloctane; Scaffold number: 12; Isomeric number: 8_2; SMILES: CC(C)C[C@@H](CCCC)C

2,5-Dimethyloctane; Scaffold number: 13; Isomeric number: 9_1; SMILES: CC(C)CC[C@H](CCC)C

2,5-Dimethyloctane; Scaffold number: 14; Isomeric number: 9_2; SMILES: CC(C)CC[C@@H](CCC)C

2,6-Dimethyloctane; Scaffold number: 15; Isomeric number: 10_1; SMILES: CC(C)CCC[C@H](CC)C

2,6-Dimethyloctane; Scaffold number: 16; Isomeric number: 10_2; SMILES: CC(C)CCC[C@@H](CC)C

2,7-Dimethyloctane; Scaffold number: 17; Isomeric number: 11; SMILES: CC(C)CCCC(C)C

3,3-Dimethyloctane; Scaffold number: 18; Isomeric number: 12; SMILES: CC(CC)(CCCCC)C

3,4-Dimethyloctane; Scaffold number: 19; Isomeric number: 13_1; SMILES: C[C@H](CC)[C@H](CCCC)C

3,4-Dimethyloctane; Scaffold number: 20; Isomeric number: 13_2; SMILES: C[C@@H](CC)[C@@H] (CCCC)C

3,4-Dimethyloctane; Scaffold number: 21; Isomeric number: 13_3; SMILES: C[C@H](CC)[C@@H](CCCC)C

3,4-Dimethyloctane; Scaffold number: 22; Isomeric number: 13_4; SMILES: C[C@@H](CC)[C@H](CCCC)C

3,5-Dimethyloctane; Scaffold number: 23; Isomeric number: 14_1; SMILES: C[C@H](CC)C[C@H](CCC)C

3,5-Dimethyloctane; Scaffold number: 24; Isomeric number: 14_2; SMILES: C[C@@H](CC)C[C@@H] (CCC)C

3,5-Dimethyloctane; Scaffold number: 25; Isomeric number: 14_3; SMILES: C[C@H](CC)C[C@@H](CCC)C

3,5-Dimethyloctane; Scaffold number: 26; Isomeric number: 14_4; SMILES: C[C@@H](CC)C[C@H](CCC)C

3,6-Dimethyloctane; Scaffold number: 27; Isomeric number: 15_1; SMILES: C[C@H](CC)CC[C@H](CC)C

3,6-Dimethyloctane; Scaffold number: 28; Isomeric number: 15_2; SMILES: C[C@@H](CC)CC[C@@H] (CC)C

3,6-Dimethyloctane; Scaffold number: 29; Isomeric number: 15_3; SMILES: C[C@H](CC)CC[C@@H](CC)C

3,6-Dimethyloctane; Scaffold number: 30; Isomeric number: 15_4; SMILES: C[C@@H](CC)CC[C@H](CC)C

4,4-Dimethyloctane; Scaffold number: 31; Isomeric number: 16; SMILES: CC(CCC)(CCCC)C

4,5-Dimethyloctane; Scaffold number: 32; Isomeric number: 17_1; SMILES: C[C@H](CCC)[C@H](CCC)C

4,5-Dimethyloctane; Scaffold number: 33; Isomeric number: 17_2; SMILES: C[C@@H](CCC)[C@@H] (CCC)C

4,5-Dimethyloctane; Scaffold number: 34; Isomeric number: 17_3; SMILES: C[C@H](CCC)[C@@H](CCC)C

4,5-Dimethyloctane; Scaffold number: 35; Isomeric number: 17_4; SMILES: C[C@@H](CCC)[C@H](CCC)C

3-Ethyloctane; Scaffold number: 36; Isomeric number: 18; SMILES: C(C)C(CC)CCCC

4-Ethyloctane; Scaffold number: 37; Isomeric number: 19_1; SMILES: C(C)[C@H](CCC)CCC

4-Ethyloctane; Scaffold number: 38; Isomeric number: 19_2; SMILES: C(C)[C@@H](CCC)CCCC

2,2,3-Trimethylheptane; Scaffold number: 39; Isomeric number: 20_1; SMILES: CC(C)([C@H](CCCC)C)C

2,2,3-Trimethylheptane; Scaffold number: 40; Isomeric number: 20_2; SMILES: CC(C)([C@@H](CCCC)C)C

2,2,4-Trimethylheptane; Scaffold number: 41; Isomeric number: 21_1; SMILES: CC(C)(C[C@H](CCC)C)C

2,2,4-Trimethylheptane; Scaffold number: 42; Isomeric number: 21_2; SMILES: CC(C)(C[C@@H](CCC)C)C

2,2,5-Trimethylheptane; Scaffold number: 43; Isomeric number: 22_1; SMILES: CC(C)(CC[C@H](CC)C)C

2,2,5-Trimethylheptane; Scaffold number: 44; Isomeric number: 22_2; SMILES: CC(C)(CC[C@@H](CC)C)C

2,2,6-Trimethylheptane; Scaffold number: 45; Isomeric number: 23; SMILES: CC(C)(CCCC(C)C)C

2,3,3-Trimethylheptane; Scaffold number: 46; Isomeric number: 24; SMILES: CC(C)C(CCC)(C)C

2,3,4-Trimethylheptane; Scaffold number: 47; Isomeric number: 25_1; SMILES: CC(C)[C@H]([C@H] (CCC)C)C

2,3,4-Trimethylheptane; Scaffold number: 48; Isomeric number: 25_2; SMILES: CC(C)[C@@H]([C@@H](CCC)C)C

2,3,4-Trimethylheptane; Scaffold number: 49; Isomeric number: 25_3; SMILES: CC(C)[C@H]([C@@H] (CCC)C)C

2,3,4-Trimethylheptane; Scaffold number: 50; Isomeric number: 25_4 ; SMILES: CC(C)[C@@H]([C@H] (CCC)C)C

2,3,5-Trimethylheptane; Scaffold number: 51; Isomeric number: 26_1; SMILES: CC(C)[C@H](C[C@H](CC)C)C

2,3,5-Trimethylheptane; Scaffold number: 52; Isomeric number: 26_2; SMILES: CC(C)[C@@H](C[C@@H](CC)C)C

2,3,5-Trimethylheptane; Scaffold number: 53; Isomeric number: 26_3; SMILES: CC(C)[C@H](C[C@@H](CC)C)C

2,3,5-Trimethylheptane; Scaffold number: 54; Isomeric number: 26_4; SMILES: CC(C)[C@@H](C[C@H] (CC)C)C

2,3,6-Trimethylheptane; Scaffold number: 55; Isomeric number: 27_1; SMILES: CC(C)[C@H](CCC(C)C)C

2,3,6-Trimethylheptane; Scaffold number: 56; Isomeric number: 27_2; SMILES: CC(C)[C@@H](CCC(C)C)C

2,4,4-Trimethylheptane; Scaffold number: 57; Isomeric number: 28; SMILES: CC(C)CC(CCC)(C)C

2,4,5-Trimethylheptane; Scaffold number: 58; Isomeric number: 29_1; SMILES: CC(C)C[C@H]([C@H] (CC)C)C

2,4,5-Trimethylheptane; Scaffold number: 59; Isomeric number: 29_2; SMILES: CC(C)C[C@@H]([C@@H] (CC)C)C

2,4,5-Trimethylheptane; Scaffold number: 60; Isomeric number: 29_3; SMILES: CC(C)C[C@H]([C@@H] (CC)C)C

2,4,5-Trimethylheptane; Scaffold number: 61; Isomeric number: 29_4; SMILES: CC(C)C[C@@H]([C@H] (CC)C)C

2,4,6-Trimethylheptane; Scaffold number: 62; Isomeric number: 30; SMILES: CC(C)CC(CC(C)C)C

2,5,5-Trimethylheptane; Scaffold number: 63; Isomeric number: 31; SMILES: CC(C)CCC(CC)(C)C

3,3,4-Trimethylheptane; Scaffold number: 64; Isomeric number: 32_1; SMILES: CC(CC)([C@H](CCC)C)C

3,3,4-Trimethylheptane; Scaffold number: 65; Isomeric number: 32_2; SMILES: CC(CC)([C@@H](CCC)C)C

3,3,5-Trimethylheptane; Scaffold number: 66; Isomeric number: 33_1; SMILES: CC(CC)(C[C@H](CC)C)C

3,3,5-Trimethylheptane; Scaffold number: 67; Isomeric number: 33_2; SMILES: CC(CC)(C[C@@H](CC)C)C

3,4,4-Trimethylheptane; Scaffold number: 68; Isomeric number: 34_1; SMILES: C[C@H](CC)C(CCC)(C)C

3,4,4-Trimethylheptane; Scaffold number: 69; Isomeric number: 34_2; SMILES: C[C@@H](CC)C(CCC)(C)C

3,4,5-Trimethylheptane; Scaffold number: 70; Isomeric number: 35_1; SMILES: C[C@H](CC)[C@H]([C@H](CC)C)C

3,4,5-Trimethylheptane; Scaffold number: 71; Isomeric number: 35_2; SMILES: C[C@H](CC)[C@H] ([C@@H](CC)C)C

3,4,5-Trimethylheptane; Scaffold number: 72; Isomeric number: 35_3; SMILES: C[C@H](CC)[C@@H] ([C@@H](CC)C)C

3,4,5-Trimethylheptane; Scaffold number: 73; Isomeric number: 35_4; SMILES: C[C@@H](CC)[C@H] ([C@H](CC)C)C

3,4,5-Trimethylheptane; Scaffold number: 74; Isomeric number: 35_5; SMILES: C[C@@H](CC)[C@@H] ([C@H](CC)C)C

3,4,5-Trimethylheptane; Scaffold number: 75; Isomeric number: 35_6; SMILES: C[C@@H](CC)[C@@H] ([C@@H](CC)C)C

3,4,5-Trimethylheptane; Scaffold number: 76; Isomeric number: 35_7; SMILES: C[C@H](CC)[C@@H] ([C@H](CC)C)C

3,4,5-Trimethylheptane; Scaffold number: 77; Isomeric number: 35_8; SMILES: C[C@@H](CC)[C@H] ([C@@H](CC)C)C

3-Ethyl-2-methylheptane; Scaffold number: 78; Isomeric number: 36_1; SMILES: C(C)[C@H](C(C)C)CCCC

3-Ethyl-2-methylheptane; Scaffold number: 79; Isomeric number: 36_2; SMILES: C(C)[C@@H](C(C)C)CCCC

3-Ethyl-3-methylheptane; Scaffold number: 80; Isomeric number: 37; SMILES: C(C)C(CC)(CCC)C

3-Ethyl-4-methylheptane; Scaffold number: 81; Isomeric number: 38_1; SMILES: C(C)C(CC)[C@H](CCC)C

3-Ethyl-4-methylheptane; Scaffold number: 82; Isomeric number: 38_2; SMILES: C(C)C(CC)[C@@H](CCC)C

3-Ethyl-5-methylheptane; Scaffold number: 83; Isomeric number: 39_1; SMILES: C(C)C(CC)C[C@H](CC)C

3-Ethyl-5-methylheptane; Scaffold number: 84; Isomeric number: 39_2; SMILES: C(C)C(CC)C[C@@H](CC)C

 $4-Ethyl-2-methylheptane; Scaffold number: 85; Isomeric number: 40_1; SMILES: C(C)[C@H](CC(C)C)CCC \\$

4-Ethyl-2-methylheptane; Scaffold number: 86; Isomeric number: 40_2; SMILES: C(C)[C@@H](CC(C)C)CCC

4-Ethyl-3-methylheptane; Scaffold number: 87; Isomeric number: 41_1; SMILES: C(C)[C@H]([C@H] (CC)C)CCC

4-Ethyl-3-methylheptane; Scaffold number: 88; Isomeric number: 41_2; SMILES: C(C)[C@@H]([C@@H] (CC)C)CCC

4-Ethyl-3-methylheptane; Scaffold number: 89; Isomeric number: 41_3; SMILES: C(C)[C@H]([C@@H] (CC)C)CCC

4-Ethyl-3-methylheptane; Scaffold number: 90; Isomeric number: 41_4; SMILES: C(C)[C@@H]([C@H] (CC)C)CCC

4-Ethyl-4-methylheptane; Scaffold number: 91; Isomeric number: 42; SMILES: C(C)C(CCC)(CCC)C

5-Ethyl-2-methylheptane; Scaffold number: 92; Isomeric number: 43; SMILES: C(C)C(CCC(C)C)CC

4-Propylheptane; Scaffold number: 93; Isomeric number: 44; SMILES: C(CC)C(CCC)CCC

4-(1-Methylethyl)heptane; Scaffold number: 94; Isomeric number: 45; SMILES: CC(C)C(CCC)CCC

2,2,3,3-Tetramethylhexane; Scaffold number: 95; Isomeric number: 46; SMILES: CC(C)(C(CCC)(C)C)C

2,2,3,4-Tetramethylhexane; Scaffold number: 96; Isomeric number: 47_1; SMILES: CC(C)([C@H]([C@H] (CC)C)C)C

2,2,3,4-Tetramethylhexane; Scaffold number: 97; Isomeric number: 47_2 ; SMILES: CC(C)([C@@H]([C@@H](CC)C)C)C

2,2,3,4-Tetramethylhexane; Scaffold number: 98; Isomeric number: 47_3 ; SMILES: CC(C)([C@H]([C@@H](CC)C)C)C

2,2,3,4-Tetramethylhexane; Scaffold number: 99; Isomeric number: 47_4; SMILES: CC(C)([C@@H]([C@H] (CC)C)C)C

2,2,3,5-Tetramethylhexane; Scaffold number: 100; Isomeric number: 48_1 ; SMILES: CC(C)([C@H](CC(C)C)C)

2,2,3,5-Tetramethylhexane; Scaffold number: 101; Isomeric number: 48_2; SMILES: CC(C)([C@@H] (CC(C)C)C)C

2,2,4,4-Tetramethylhexane; Scaffold number: 102; Isomeric number: 49; SMILES: CC(C)(CC(CC)(C)C)C

2,2,4,5-Tetramethylhexane; Scaffold number: 103; Isomeric number: 50_1 ; SMILES: CC(C)(C[C@H](C(C)C)C)

2,2,4,5-Tetramethylhexane; Scaffold number: 104; Isomeric number: 50_2; SMILES: CC(C)(C[C@@H] (C(C)C)C)C

2,2,5,5-Tetramethylhexane; Scaffold number: 105; Isomeric number: 51; SMILES: CC(C)(CCC(C)(C)C)C

2,3,3,4-Tetramethylhexane; Scaffold number: 106; Isomeric number: 52_1 ; SMILES: CC(C)C([C@H](CC)C) (C)C

2,3,3,4-Tetramethylhexane; Scaffold number: 107; Isomeric number: 52_2; SMILES: CC(C)C([C@@H](CC)C) (C)C

2,3,3,5-Tetramethylhexane; Scaffold number: 108; Isomeric number: 53; SMILES: CC(C)C(CC(C)C)(C)C

2,3,4,4-Tetramethylhexane; Scaffold number: 109; Isomeric number: 54_1; SMILES: CC(C)[C@H](C(CC) (C)C)C

2,3,4,4-Tetramethylhexane; Scaffold number: 110; Isomeric number: 54_2; SMILES: CC(C)[C@@H](C(CC) (C)C)C

2,3,4,5-Tetramethylhexane; Scaffold number: 111; Isomeric number: 55_1; SMILES: CC(C)[C@H]([C@H] (C(C)C)C)C

2,3,4,5-Tetramethylhexane; Scaffold number: 112; Isomeric number: 55_2; SMILES: CC(C)[C@@H]([C@@H] (C(C)C)C)C

2,3,4,5-Tetramethylhexane; Scaffold number: 113; Isomeric number: 55_3; SMILES: CC(C)[C@H]([C@@H] (C(C)C)C)C

2,3,4,5-Tetramethylhexane; Scaffold number: 114; Isomeric number: 55_4; SMILES: CC(C)[C@@H]([C@H] (C(C)C)C)C

3,3,4,4-Tetramethylhexane; Scaffold number: 115; Isomeric number: 56; SMILES: CC(CC)(C(CC)(C)C)C

3-Ethyl-2,2-dimethylhexane; Scaffold number: 116; Isomeric number: 57_1 ; SMILES: C(C)[C@H](C(C)(C)C)CCC

3-Ethyl-2,2-dimethylhexane; Scaffold number: 117; Isomeric number: 57_2; SMILES: C(C)[C@@H](C(C) (C)C)CCC

3-Ethyl-2,3-dimethylhexane; Scaffold number: 118; Isomeric number: 58_1; SMILES: C(C)[C@](C(C)C) (CCC)C

3-Ethyl-2,3-dimethylhexane; Scaffold number: 119; Isomeric number: 58_2 ; SMILES: C(C)[C@@](C(C)C) (CCC)C

3-Ethyl-2,4-dimethylhexane; Scaffold number: 120; Isomeric number: 59_1; SMILES: C(C)[C@H](C(C)C) [C@H](CC)C

3-Ethyl-2,4-dimethylhexane; Scaffold number: 121; Isomeric number: 59_2; SMILES: C(C)[C@@H](C(C)C) [C@@H](CC)C

3-Ethyl-2,4-dimethylhexane; Scaffold number: 122; Isomeric number: 59_3; SMILES: C(C)[C@H](C(C)C) [C@@H](CC)C

3-Ethyl-2,4-dimethylhexane; Scaffold number: 123; Isomeric number: 59_4; SMILES: C(C)[C@@H](C(C)C) [C@H](CC)C

3-Ethyl-2,5-dimethylhexane; Scaffold number: 124; Isomeric number: 60_1; SMILES: C(C)[C@H] (C(C)C)CC(C)C

3-Ethyl-2,5-dimethylhexane; Scaffold number: 125; Isomeric number: 60_2; SMILES: C(C)[C@@H] (C(C)C)CC(C)C

3-Ethyl-3,4-dimethylhexane; Scaffold number: 126; Isomeric number: 61_1; SMILES: C(C)C(CC)([C@H] (CC)C)C

3-Ethyl-3,4-dimethylhexane; Scaffold number: 127; Isomeric number: 61_2; SMILES: C(C)C(CC)([C@@H] (CC)C)C

4-Ethyl-2,2-dimethylhexane; Scaffold number: 128; Isomeric number: 62; SMILES: C(C)C(CC(C)(C)C)CC

4-Ethyl-2,3-dimethylhexane; Scaffold number: 129; Isomeric number: 63_1; SMILES: C(C)C([C@H] (C(C)C)C)CC

4-Ethyl-2,3-dimethylhexane; Scaffold number: 130; Isomeric number: 63_2; SMILES: C(C)C([C@@H](C(C)C)C)CC

4-Ethyl-2,4-dimethylhexane; Scaffold number: 131; Isomeric number: 64; SMILES: C(C)C(CC(C)C)(CC)C

4-Ethyl-3,3-dimethylhexane; Scaffold number: 132; Isomeric number: 65; SMILES: C(C)C(C(CC)C)CC

3,3-Diethylhexane; Scaffold number: 133; Isomeric number: 66; SMILES: C(C)C(CC)(CCC)CC

3,4-Diethylhexane; Scaffold number: 134; Isomeric number: 67; SMILES: C(C)C(CC)C(CC)CC

2-Methyl-3-(1-methylethyl)hexane; Scaffold number: 135; Isomeric number: 68; SMILES: CC(C)C(CCC)C(C)C

$$\begin{array}{c|c} H_3C & CH_3 \\ \hline \\ CH_3 & CH_3 \\ \hline \end{array}$$

2,2,3,3,4-Pentamethylpentane; Scaffold number: 136; Isomeric number: 69; SMILES: CC(C)(C(C)C)(C)C)C

2,2,3,4,4-Pentamethylpentane; Scaffold number: 137; Isomeric number: 70; SMILES: CC(C)(C(C)(C)C)C)C

3-Ethyl-2,2,4-trimethylpentane; Scaffold number: 139; Isomeric number: 72_1; SMILES: C(C)[C@H](C(C) (C)C)C(C)C

3-Ethyl-2,2,4-trimethylpentane; Scaffold number: 140; Isomeric number: 72_2; SMILES: C(C)[C@@H](C(C) (C)C)C(C)C

3-Ethyl-2,3,4-trimethylpentane; Scaffold number: 141; Isomeric number: 73; SMILES: C(C)C(C(C)C)(C(C)C)C

3,3-Diethyl-2-methylpentane; Scaffold number: 142; Isomeric number: 74; SMILES: C(C)C(C(C)C)(CC)CC

2,4-Dimethyl-3-(1-methylethyl)pentane; Scaffold number: 143; Isomeric number: 75; SMILES: CC(C)C(C(C)C)C