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| Decane; Scaffold number: 1; Isomeric number: 1; SMILES: CCCCCCCCCC |
| 2-Methylnonane; Scaffold number: 2; Isomeric number: 2; SMILES: CC(C)CCCCCCC |
| 3-Methylnonane; Scaffold number: 3; Isomeric number: 3\_1; SMILES: C[C@H](CC)CCCCCC |
| 3-Methylnonane; Scaffold number: 4; Isomeric number: 3\_2; SMILES: C[C@@H](CC)CCCCCC |
| 4-Methylnonane; Scaffold number: 5; Isomeric number: 4\_1; SMILES: C[C@H](CCC)CCCCC |
| 4-Methylnonane; Scaffold number: 6; Isomeric number: 4\_2; SMILES: C[C@@H](CCC)CCCCC |
| 5-Methylnonane; Scaffold number: 7; Isomeric number: 5; SMILES: CC(CCCC)CCCC |
| 2,2-Dimethyloctane; Scaffold number: 8; Isomeric number: 6; SMILES: CC(C)(CCCCCC)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 |
| 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)CCCCC(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)CCCCC |
| 4-Ethyloctane; Scaffold number: 37; Isomeric number: 19\_1; SMILES: C(C)[C@H](CCC)CCCC |
| 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(CCCC)(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)(CCCC)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)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)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)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 |
| 2,2,3,3,4-Pentamethylpentane; Scaffold number: 136; Isomeric number: 69; SMILES: CC(C)(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)C |
| 3-Ethyl-2,2,3-trimethylpentane; Scaffold number: 138; Isomeric number: 71; SMILES: C(C)C(C(C)(C)C)(CC)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(C)C |