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| Decane; scaffold number: 1; chiral centres: 1; SMILES: CCCCCCCCCC |
| 2-Methylnonane; scaffold number: 2; chiral centres: 1; SMILES: CC(C)CCCCCCC |
| 3-Methylnonane; scaffold number: 3; chiral centres: 2; SMILES: CC(CC)CCCCCC |
| 4-Methylnonane; scaffold number: 4; chiral centres: 2; SMILES: CC(CCC)CCCCC |
| 5-Methylnonane; scaffold number: 5; chiral centres: 1; SMILES: CC(CCCC)CCCC |
| 2,2-Dimethyloctane; scaffold number: 6; chiral centres: 1; SMILES: CC(C)(CCCCCC)C |
| 2,3-Dimethyloctane; scaffold number: 7; chiral centres: 2; SMILES: CC(C)C(CCCCC)C |
| 2,4-Dimethyloctane; scaffold number: 8; chiral centres: 2; SMILES: CC(C)CC(CCCC)C |
| 2,5-Dimethyloctane; scaffold number: 9; chiral centres: 2; SMILES: CC(C)CCC(CCC)C |
| 2,6-Dimethyloctane; scaffold number: 10; chiral centres: 2; SMILES: CC(C)CCCC(CC)C |
| 2,7-Dimethyloctane; scaffold number: 11; chiral centres: 1; SMILES: CC(C)CCCCC(C)C |
| 3,3-Dimethyloctane; scaffold number: 12; chiral centres: 1; SMILES: CC(CC)(CCCCC)C |
| 3,4-Dimethyloctane; scaffold number: 13; chiral centres: 4; SMILES: CC(CC)C(CCCC)C |
| 3,5-Dimethyloctane; scaffold number: 14; chiral centres: 4; SMILES: CC(CC)CC(CCC)C |
| 3,6-Dimethyloctane; scaffold number: 15; chiral centres: 4; SMILES: CC(CC)CCC(CC)C |
| 4,4-Dimethyloctane; scaffold number: 16; chiral centres: 1; SMILES: CC(CCC)(CCCC)C |
| 4,5-Dimethyloctane; scaffold number: 17; chiral centres: 4; SMILES: CC(CCC)C(CCC)C |
| 3-Ethyloctane; scaffold number: 18; chiral centres: 1; SMILES: C(C)C(CC)CCCCC |
| 4-Ethyloctane; scaffold number: 19; chiral centres: 2; SMILES: C(C)C(CCC)CCCC |
| 2,2,3-Trimethylheptane; scaffold number: 20; chiral centres: 2; SMILES: CC(C)(C(CCCC)C)C |
| 2,2,4-Trimethylheptane; scaffold number: 21; chiral centres: 2; SMILES: CC(C)(CC(CCC)C)C |
| 2,2,5-Trimethylheptane; scaffold number: 22; chiral centres: 2; SMILES: CC(C)(CCC(CC)C)C |
| 2,2,6-Trimethylheptane; scaffold number: 23; chiral centres: 1; SMILES: CC(C)(CCCC(C)C)C |
| 2,3,3-Trimethylheptane; scaffold number: 24; chiral centres: 1; SMILES: CC(C)C(CCCC)(C)C |
| 2,3,4-Trimethylheptane; scaffold number: 25; chiral centres: 4; SMILES: CC(C)C(C(CCC)C)C |
| 2,3,5-Trimethylheptane; scaffold number: 26; chiral centres: 4; SMILES: CC(C)C(CC(CC)C)C |
| 2,3,6-Trimethylheptane; scaffold number: 27; chiral centres: 2; SMILES: CC(C)C(CCC(C)C)C |
| 2,4,4-Trimethylheptane; scaffold number: 28; chiral centres: 1; SMILES: CC(C)CC(CCC)(C)C |
| 2,4,5-Trimethylheptane; scaffold number: 29; chiral centres: 4; SMILES: CC(C)CC(C(CC)C)C |
| 2,4,6-Trimethylheptane; scaffold number: 30; chiral centres: 1; SMILES: CC(C)CC(CC(C)C)C |
| 2,5,5-Trimethylheptane; scaffold number: 31; chiral centres: 1; SMILES: CC(C)CCC(CC)(C)C |
| 3,3,4-Trimethylheptane; scaffold number: 32; chiral centres: 2; SMILES: CC(CC)(C(CCC)C)C |
| 3,3,5-Trimethylheptane; scaffold number: 33; chiral centres: 2; SMILES: CC(CC)(CC(CC)C)C |
| 3,4,4-Trimethylheptane; scaffold number: 34; chiral centres: 2; SMILES: CC(CC)C(CCC)(C)C |
| 3,4,5-Trimethylheptane; scaffold number: 35; chiral centres: 8; SMILES: CC(CC)C(C(CC)C)C |
| 3-Ethyl-2-methylheptane; scaffold number: 36; chiral centres: 2; SMILES: C(C)C(C(C)C)CCCC |
| 3-Ethyl-3-methylheptane; scaffold number: 37; chiral centres: 1; SMILES: C(C)C(CC)(CCCC)C |
| 3-Ethyl-4-methylheptane; scaffold number: 38; chiral centres: 2; SMILES: C(C)C(CC)C(CCC)C |
| 3-Ethyl-5-methylheptane; scaffold number: 39; chiral centres: 2; SMILES: C(C)C(CC)CC(CC)C |
| 4-Ethyl-2-methylheptane; scaffold number: 40; chiral centres: 2; SMILES: C(C)C(CC(C)C)CCC |
| 4-Ethyl-3-methylheptane; scaffold number: 41; chiral centres: 4; SMILES: C(C)C(C(CC)C)CCC |
| 4-Ethyl-4-methylheptane; scaffold number: 42; chiral centres: 1; SMILES: C(C)C(CCC)(CCC)C |
| 5-Ethyl-2-methylheptane; scaffold number: 43; chiral centres: 1; SMILES: C(C)C(CCC(C)C)CC |
| 4-Propylheptane; scaffold number: 44; chiral centres: 1; SMILES: C(CC)C(CCC)CCC |
| 4-(1-Methylethyl)heptane; scaffold number: 45; chiral centres: 1; SMILES: CC(C)C(CCC)CCC |
| 2,2,3,3-Tetramethylhexane; scaffold number: 46; chiral centres: 1; SMILES: CC(C)(C(CCC)(C)C)C |
| 2,2,3,4-Tetramethylhexane; scaffold number: 47; chiral centres: 4; SMILES: CC(C)(C(C(CC)C)C)C |
| 2,2,3,5-Tetramethylhexane; scaffold number: 48; chiral centres: 2; SMILES: CC(C)(C(CC(C)C)C)C |
| 2,2,4,4-Tetramethylhexane; scaffold number: 49; chiral centres: 1; SMILES: CC(C)(CC(CC)(C)C)C |
| 2,2,4,5-Tetramethylhexane; scaffold number: 50; chiral centres: 2; SMILES: CC(C)(CC(C(C)C)C)C |
| 2,2,5,5-Tetramethylhexane; scaffold number: 51; chiral centres: 1; SMILES: CC(C)(CCC(C)(C)C)C |
| 2,3,3,4-Tetramethylhexane; scaffold number: 52; chiral centres: 2; SMILES: CC(C)C(C(CC)C)(C)C |
| 2,3,3,5-Tetramethylhexane; scaffold number: 53; chiral centres: 1; SMILES: CC(C)C(CC(C)C)(C)C |
| 2,3,4,4-Tetramethylhexane; scaffold number: 54; chiral centres: 2; SMILES: CC(C)C(C(CC)(C)C)C |
| 2,3,4,5-Tetramethylhexane; scaffold number: 55; chiral centres: 4; SMILES: CC(C)C(C(C(C)C)C)C |
| 3,3,4,4-Tetramethylhexane; scaffold number: 56; chiral centres: 1; SMILES: CC(CC)(C(CC)(C)C)C |
| 3-Ethyl-2,2-dimethylhexane; scaffold number: 57; chiral centres: 2; SMILES: C(C)C(C(C)(C)C)CCC |
| 3-Ethyl-2,3-dimethylhexane; scaffold number: 58; chiral centres: 2; SMILES: C(C)C(C(C)C)(CCC)C |
| 3-Ethyl-2,4-dimethylhexane; scaffold number: 59; chiral centres: 4; SMILES: C(C)C(C(C)C)C(CC)C |
| 3-Ethyl-2,5-dimethylhexane; scaffold number: 60; chiral centres: 2; SMILES: C(C)C(C(C)C)CC(C)C |
| 3-Ethyl-3,4-dimethylhexane; scaffold number: 61; chiral centres: 2; SMILES: C(C)C(CC)(C(CC)C)C |
| 4-Ethyl-2,2-dimethylhexane; scaffold number: 62; chiral centres: 1; SMILES: C(C)C(CC(C)(C)C)CC |
| 4-Ethyl-2,3-dimethylhexane; scaffold number: 63; chiral centres: 2; SMILES: C(C)C(C(C(C)C)C)CC |
| 4-Ethyl-2,4-dimethylhexane; scaffold number: 64; chiral centres: 1; SMILES: C(C)C(CC(C)C)(CC)C |
| 4-Ethyl-3,3-dimethylhexane; scaffold number: 65; chiral centres: 1; SMILES: C(C)C(C(CC)(C)C)CC |
| 3,3-Diethylhexane; scaffold number: 66; chiral centres: 1; SMILES: C(C)C(CC)(CCC)CC |
| 3,4-Diethylhexane; scaffold number: 67; chiral centres: 1; SMILES: C(C)C(CC)C(CC)CC |
| 2-Methyl-3-(1-methylethyl)hexane; scaffold number: 68; chiral centres: 1; SMILES: CC(C)C(CCC)C(C)C |
| 2,2,3,3,4-Pentamethylpentane; scaffold number: 69; chiral centres: 1; SMILES: CC(C)(C(C(C)C)(C)C)C |
| 2,2,3,4,4-Pentamethylpentane; scaffold number: 70; chiral centres: 1; SMILES: CC(C)(C(C(C)(C)C)C)C |
| 3-Ethyl-2,2,3-trimethylpentane; scaffold number: 71; chiral centres: 1; SMILES: C(C)C(C(C)(C)C)(CC)C |
| 3-Ethyl-2,2,4-trimethylpentane; scaffold number: 72; chiral centres: 2; SMILES: C(C)C(C(C)(C)C)C(C)C |
| 3-Ethyl-2,3,4-trimethylpentane; scaffold number: 73; chiral centres: 1; SMILES: C(C)C(C(C)C)(C(C)C)C |
| 3,3-Diethyl-2-methylpentane; scaffold number: 74; chiral centres: 1; SMILES: C(C)C(C(C)C)(CC)CC |
| 2,4-Dimethyl-3-(1-methylethyl)pentane; scaffold number: 75; chiral centres: 1; SMILES: CC(C)C(C(C)C)C(C)C |