

(3aS,5S,8S)-3a-Hydroxy-1,5,8-trimethyl-4,5,8,9-tetrahydronaphthalen-1-one

Inchi:	InChI=1S/C15H18O4/c1-7-4-10-12(11(16)5-7)8(2)6-15(18)13(10)9(3)14(17)19-15/h7-8,11,13,14,16,17,19-20,22-23,25-26,28-29,31-32,34-35,37-38,40-41,43-44,46-47,49-50,52-53,55-56,58-59,61-62,64-65,67-68,70-71,73-74,76-77,79-80,82-83,85-86,88-89,91-92,94-95,97-98,100-101,103-104,106-107,109-110,112-113,115-116,118-119,121-122,124-125,127-128,130-131,133-134,136-137,139-140,142-143,145-146,148-149,151-152,154-155,157-158,160-161,163-164,166-167,169-170,172-173,175-176,178-179,181-182,184-185,187-188,190-191,193-194,196-197,199-200,202-203,205-206,208-209,211-212,214-215,217-218,220-221,223-224,226-227,229-230,232-233,235-236,238-239,241-242,244-245,247-248,250-251,253-254,256-257,259-260,262-263,265-266,268-269,271-272,274-275,277-278,280-281,283-284,286-287,289-290,292-293,295-296,298-299,301-302,304-305,307-308,310-311,313-314,316-317,319-320,322-323,325-326,328-329,331-332,334-335,337-338,340-341,343-344,346-347,349-350,352-353,355-356,358-359,361-362,364-365,367-368,370-371,373-374,376-377,379-380,382-383,385-386,388-389,391-392,394-395,397-398,399,401-402,404-405,407-408,410-411,413-414,416-417,419-420,422-423,425-426,428-429,431-432,434-435,437-438,440-441,443-444,446-447,449-450,452-453,455-456,458-459,461-462,464-465,467-468,470-471,473-474,476-477,479-480,482-483,485-486,488-489,491-492,494-495,497-498,499,501-502,504-505,507-508,510-511,513-514,516-517,519-520,522-523,525-526,528-529,531-532,534-535,537-538,540-541,543-544,546-547,549-550,552-553,555-556,558-559,561-562,564-565,567-568,570-571,573-574,576-577,579-580,582-583,585-586,588-589,591-592,594-595,597-598,599,601-602,604-605,607-608,610-611,613-614,616-617,619-620,622-623,625-626,628-629,631-632,634-635,637-638,640-641,643-644,646-647,649-650,652-653,655-656,658-659,661-662,664-665,667-668,670-671,673-674,676-677,679-680,682-683,685-686,688-689,691-692,694-695,697-698,699,701-702,704-705,707-708,710-711,713-714,716-717,719-720,722-723,725-726,728-729,731-732,734-735,737-738,740-741,743-744,746-747,749-750,752-753,755-756,758-759,761-762,764-765,767-768,770-771,773-774,776-777,779-780,782-783,785-786,788-789,791-792,794-795,797-798,799,801-802,804-805,807-808,810-811,813-814,816-817,819-820,822-823,825-826,828-829,831-832,834-835,837-838,840-841,843-844,846-847,849-850,852-853,855-856,858-859,861-862,864-865,867-868,870-871,873-874,876-877,879-880,882-883,885-886,888-889,891-892,894-895,897-898,899,901-902,904-905,907-908,910-911,913-914,916-917,919-920,922-923,925-926,928-929,931-932,934-935,937-938,940-941,943-944,946-947,949-950,952-953,955-956,958-959,961-962,964-965,967-968,970-971,973-974,976-977,979-980,982-983,985-986,988-989,991-992,994-995,997-998,999,1001-1002,1004-1005,1007-1008,1010-1011,1013-1014,1016-1017,1019-1020,1022-1023,1025-1026,1028-1029,1031-1032,1034-1035,1037-1038,1040-1041,1043-1044,1046-1047,1049-1050,1052-1053,1055-1056,1058-1059,1061-1062,1064-1065,1067-1068,1070-1071,1073-1074,1076-1077,1079-1080,1082-1083,1085-1086,1088-1089,1091-1092,1094-1095,1097-1098,1099,1101-1102,1104-1105,1107-1108,1110-1111,1113-1114,1116-1117,1119-1120,1122-1123,1125-1126,1128-1129,1131-1132,1134-1135,1137-1138,1140-1141,1143-1144,1146-1147,1149-1150,1152-1153,1155-1156,1158-1159,1161-1162,1164-1165,1167-1168,1170-1171,1173-1174,1176-1177,1179-1180,1182-1183,1185-1186,1188-1189,1191-1192,1194-1195,1197-1198,1199,1201-1202,1204-1205,1207-1208,1210-1211,1213-1214,1216-1217,1219-1220,1222-1223,1225-1226,1228-1229,1231-1232,1234-1235,1237-1238,1240-1241,1243-1244,1246-1247,1249-1250,1252-1253,1255-1256,1258-1259,1261-1262,1264-1265,1267-1268,1270-1271,1273-1274,1276-1277,1279-1280,1282-1283,1285-1286,1288-1289,1291-1292,1294-1295,1297-1298,1299,1301-1302,1304-1305,1307-1308,1310-1311,1313-1314,1316-1317,1319-1320,1322-1323,1325-1326,1328-1329,1331-1332,1334-1335,1337-1338,1340-1341,1343-1344,1346-1347,1349-1350,1352-1353,1355-1356,1358-1359,1361-1362,1364-1365,1367-1368,1370-1371,1373-1374,1376-1377,1379-1380,1382-1383,1385-1386,1388-1389,1391-1392,1394-1395,1397-1398,1399,1401-1402,1404-1405,1407-1408,1410-1411,1413-1414,1416-1417,1419-1420,1422-1423,1425-1426,1428-1429,1431-1432,1434-1435,1437-1438,1440-1441,1443-1444,1446-1447,1449-1450,1452-1453,1455-1456,1458-1459,1461-1462,1464-1465,1467-1468,1470-1471,1473-1474,1476-1477,1479-1480,1482-1483,1485-1486,1488-1489,1491-1492,1494-1495,1497-1498,1499,1501-1502,1504-1505,1507-1508,1510-1511,1513-1514,1516-1517,1519-1520,1522-1523,1525-1526,1528-1529,1531-1532,1534-1535,1537-1538,1540-1541,1543-1544,1546-1547,1549-1550,1552-1553,1555-1556,1558-1559,1561-1562,1564-1565,1567-1568,1570-1571,1573-1574,1576-1577,1579-1580,1582-1583,1585-1586,1588-1589,1591-1592,1594-1595,1597-1598,1599,1601-1602,1604-1605,1607-1608,1610-1611,1613-1614,1616-1617,1619-1620,1622-1623,1625-1626,1628-1629,1631-1632,1634-1635,1637-1638,1640-1641,1643-1644,1646-1647,1649-1650,1652-1653,1655-1656,1658-1659,1661-1662,1664-1665,1667-1668,1670-1671,1673-1674,1676-1677,1679-1680,1682-1683,1685-1686,1688-1689,1691-1692,1694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Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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