

Succinic acid, 3-methylbut-2-yl 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C18H30O4/c1-7-8-9-16(12-13(2)3)22-18(20)11-10-17(19)21-15(6)14(4)5/h13-14,16-17,20-21,22-23,25-26,28-29,31-32,34-35,37-38,40-41,43-44,46-47,49-50,52-53,55-56,58-59,61-62,64-65,67-68,70-71,73-74,76-77,79-80,82-83,85-86,88-89,91-92,94-95,97-98,100-101,103-104,106-107,109-110,112-113,115-116,118-119,121-122,124-125,127-128,130-131,133-134,136-137,139-140,142-143,145-146,148-149,151-152,154-155,157-158,160-161,163-164,166-167,169-170,172-173,175-176,178-179,181-182,184-185,187-188,190-191,193-194,196-197,199-200,202-203,205-206,208-209,211-212,214-215,217-218,220-221,223-224,226-227,229-230,232-233,235-236,238-239,241-242,244-245,247-248,250-251,253-254,256-257,259-260,262-263,265-266,268-269,271-272,274-275,277-278,280-281,283-284,286-287,289-290,292-293,295-296,298-299,301-302,304-305,307-308,310-311,313-314,316-317,319-320,322-323,325-326,328-329,331-332,334-335,337-338,340-341,343-344,346-347,349-350,352-353,355-356,358-359,361-362,364-365,367-368,370-371,373-374,376-377,379-380,382-383,385-386,388-389,391-392,394-395,397-398,400-401,403-404,406-407,409-410,412-413,415-416,418-419,421-422,424-425,427-428,430-431,433-434,436-437,439-440,442-443,445-446,448-449,451-452,454-455,457-458,460-461,463-464,466-467,469-470,472-473,475-476,478-479,481-482,484-485,487-488,490-491,493-494,496-497,499-500,502-503,505-506,508-509,511-512,514-515,517-518,520-521,523-524,526-527,529-530,532-533,535-536,538-539,541-542,544-545,547-548,550-551,553-554,556-557,559-560,562-563,565-566,568-569,571-572,574-575,577-578,580-581,583-584,586-587,589-590,592-593,595-596,598-599,601-602,604-605,607-608,610-611,613-614,616-617,619-620,622-623,625-626,628-629,631-632,634-635,637-638,640-641,643-644,646-647,649-650,652-653,655-656,658-659,661-662,664-665,667-668,669-670,672-673,675-676,678-679,681-682,684-685,687-688,690-691,693-694,696-697,699-700,702-703,705-706,708-709,711-712,714-715,717-718,720-721,723-724,726-727,729-730,732-733,735-736,738-739,741-742,744-745,747-748,750-751,753-754,756-757,759-760,762-763,765-766,768-769,771-772,774-775,777-778,780-781,783-784,786-787,789-790,792-793,795-796,798-799,801-802,804-805,807-808,810-811,813-814,816-817,819-820,822-823,825-826,828-829,831-832,834-835,837-838,840-841,843-844,846-847,849-850,852-853,855-856,858-859,861-862,864-865,867-868,869-870,872-873,875-876,878-879,881-882,884-885,887-888,890-891,893-894,896-897,899-900,902-903,905-906,908-909,911-912,914-915,917-918,920-921,923-924,926-927,929-930,932-933,935-936,938-939,941-942,944-945,947-948,950-951,953-954,956-957,959-960,962-963,965-966,968-969,971-972,974-975,977-978,980-981,983-984,986-987,989-990,992-993,995-996,998-999,1000-1001,1003-1004,1006-1007,1009-1010,1012-1013,1015-1016,1018-1019,1021-1022,1024-1025,1027-1028,1030-1031,1033-1034,1036-1037,1039-1040,1042-1043,1045-1046,1048-1049,1051-1052,1054-1055,1057-1058,1060-1061,1063-1064,1066-1067,1069-1070,1072-1073,1075-1076,1078-1079,1081-1082,1084-1085,1087-1088,1090-1091,1093-1094,1096-1097,1099-1100,1102-1103,1105-1106,1108-1109,1111-1112,1114-1115,1117-1118,1120-1121,1123-1124,1126-1127,1129-1130,1132-1133,1135-1136,1138-1139,1141-1142,1144-1145,1147-1148,1150-1151,1153-1154,1156-1157,1159-1160,1162-1163,1165-1166,1168-1169,1171-1172,1174-1175,1177-1178,1180-1181,1183-1184,1186-1187,1189-1190,1192-1193,1195-1196,1198-1199,1201-1202,1204-1205,1207-1208,1210-1211,1213-1214,1216-1217,1219-1220,1222-1223,1225-1226,1228-1229,1231-1232,1234-1235,1237-1238,1240-1241,1243-1244,1246-1247,1249-1250,1252-1253,1255-1256,1258-1259,1261-1262,1264-1265,1267-1268,1269-1270,1272-1273,1275-1276,1278-1279,1281-1282,1284-1285,1287-1288,1290-1291,1293-1294,1296-1297,1299-1300,1302-1303,1305-1306,1308-1309,1311-1312,1314-1315,1317-1318,1320-1321,1323-1324,1326-1327,1329-1330,1332-1333,1335-1336,1338-1339,1341-1342,1344-1345,1347-1348,1350-1351,1353-1354,1356-1357,1359-1360,1362-1363,1365-1366,1368-1369,1371-1372,1374-1375,1377-1378,1380-1381,1383-1384,1386-1387,1389-1390,1392-1393,1395-1396,1398-1399,1401-1402,1404-1405,1407-1408,1410-1411,1413-1414,1416-1417,1419-1420,1422-1423,1425-1426,1428-1429,1431-1432,1434-1435,1437-1438,1440-1441,1443-1444,1446-1447,1449-1450,1452-1453,1455-1456,1458-1459,1461-1462,1464-1465,1467-1468,1469-1470,1472-1473,1475-1476,1478-1479,1481-1482,1484-1485,1487-1488,1490-1491,1493-1494,1496-1497,1499-1500,1502-1503,1505-1506,1508-1509,1511-1512,1514-1515,1517-1518,1520-1521,1523-1524,1526-1527,1529-1530,1532-1533,1535-1536,1538-1539,1541-1542,1544-1545,1547-1548,1550-1551,1553-1554,1556-1557,1559-1560,1562-1563,1565-1566,1568-1569,1571-1572,1574-1575,1577-1578,1580-1581,1583-1584,1586-1587,1589-1590,1592-1593,1595-1596,1598-1599,1601-1602,1604-1605,1607-1608,1610-1611,1613-1614,1616-1617,1619-1620,1622-1623,1625-1626,1628-1629,1631-1632,1634-1635,1637-1638,1640-1641,1643-1644,1646-1647,1649-1650,1652-1653,1655-1656,1658-1659,1661-1662,1664-1665,1667-1668,1669-1670,1672-1673,1675-1676,1678-1679,1681-1682,1684-1685,1687-1688,1690-1691,1693-1694,1695-1696,1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Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rinsol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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