

Succinic acid, di(3-heptyl) ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C18H34O4/c1-5-9-11-15(7-3)21-17(19)13-14-18(20)22-16(8-4)12-10-6-2/h15-17,21-22,24-25,27-28,30-31,33-34,36-37,39-40,42-43,45-46,48-49,51-52,54-55,57-58,60-61,63-64,66-67,69-70,72-73,75-76,78-79,81-82,84-85,87-88,90-91,93-94,96-97,99-100,102-103,105-106,108-109,111-112,114-115,117-118,120-121,123-124,126-127,129-130,132-133,135-136,138-139,141-142,144-145,147-148,150-151,153-154,156-157,159-160,162-163,165-166,168-169,171-172,174-175,177-178,180-181,183-184,186-187,189-190,192-193,195-196,198-199,201-202,204-205,207-208,210-211,213-214,216-217,219-220,222-223,225-226,228-229,231-232,234-235,237-238,240-241,243-244,246-247,249-250,252-253,255-256,258-259,261-262,264-265,267-268,270-271,273-274,276-277,279-280,282-283,285-286,288-289,291-292,294-295,297-298,300-301,303-304,306-307,309-310,312-313,315-316,318-319,321-322,324-325,327-328,330-331,333-334,336-337,339-340,342-343,345-346,348-349,351-352,354-355,357-358,360-361,363-364,366-367,369-370,372-373,375-376,378-379,381-382,384-385,387-388,390-391,393-394,396-397,399-400,402-403,405-406,408-409,411-412,414-415,417-418,420-421,423-424,426-427,429-430,432-433,435-436,438-439,441-442,444-445,447-448,450-451,453-454,456-457,459-460,462-463,465-466,468-469,471-472,474-475,477-478,480-481,483-484,486-487,489-490,492-493,495-496,498-499,501-502,504-505,507-508,510-511,513-514,516-517,519-520,522-523,525-526,528-529,531-532,534-535,537-538,540-541,543-544,546-547,549-550,552-553,555-556,558-559,561-562,564-565,567-568,569,571-572,574-575,577-578,580-581,583-584,586-587,589-590,592-593,595-596,598-599,601-602,604-605,607-608,610-611,613-614,616-617,619-620,622-623,625-626,628-629,631-632,634-635,637-638,640-641,643-644,646-647,649-650,652-653,655-656,658-659,661-662,664-665,667-668,669,671-672,674-675,677-678,680-681,683-684,686-687,689-690,692-693,695-696,698-699,701-702,704-705,707-708,710-711,713-714,716-717,719-720,722-723,725-726,728-729,731-732,734-735,737-738,740-741,743-744,746-747,749-750,752-753,755-756,758-759,761-762,764-765,767-768,769,771-772,774-775,777-778,780-781,783-784,786-787,789-790,792-793,795-796,798-799,801-802,804-805,807-808,810-811,813-814,816-817,819-820,822-823,825-826,828-829,831-832,834-835,837-838,840-841,843-844,846-847,849-850,852-853,855-856,858-859,861-862,864-865,867-868,869,871-872,874-875,877-878,880-881,883-884,886-887,889-890,892-893,895-896,898-899,901-902,904-905,907-908,910-911,913-914,916-917,919-920,922-923,925-926,928-929,931-932,934-935,937-938,940-941,943-944,946-947,949-950,952-953,955-956,958-959,961-962,964-965,967-968,969,971-972,974-975,977-978,980-981,983-984,986-987,989-990,992-993,995-996,998-999,1001-1002,1004-1005,1007-1008,1010-1011,1013-1014,1016-1017,1019-1020,1022-1023,1025-1026,1028-1029,1031-1032,1034-1035,1037-1038,1040-1041,1043-1044,1046-1047,1049-1050,1052-1053,1055-1056,1058-1059,1061-1062,1064-1065,1067-1068,1069,1071-1072,1074-1075,1077-1078,1080-1081,1083-1084,1086-1087,1089-1090,1092-1093,1095-1096,1098-1099,1101-1102,1104-1105,1107-1108,1110-1111,1113-1114,1116-1117,1119-1120,1122-1123,1125-1126,1128-1129,1131-1132,1134-1135,1137-1138,1140-1141,1143-1144,1146-1147,1149-1150,1152-1153,1155-1156,1158-1159,1161-1162,1164-1165,1167-1168,1169,1171-1172,1174-1175,1177-1178,1180-1181,1183-1184,1186-1187,1189-1190,1192-1193,1195-1196,1198-1199,1201-1202,1204-1205,1207-1208,1210-1211,1213-1214,1216-1217,1219-1220,1222-1223,1225-1226,1228-1229,1231-1232,1234-1235,1237-1238,1240-1241,1243-1244,1246-1247,1249-1250,1252-1253,1255-1256,1258-1259,1261-1262,1264-1265,1267-1268,1269,1271-1272,1274-1275,1277-1278,1280-1281,1283-1284,1286-1287,1289-1290,1292-1293,1295-1296,1298-1299,1301-1302,1304-1305,1307-1308,1310-1311,1313-1314,1316-1317,1319-1320,1322-1323,1325-1326,1328-1329,1331-1332,1334-1335,1337-1338,1340-1341,1343-1344,1346-1347,1349-1350,1352-1353,1355-1356,1358-1359,1361-1362,1364-1365,1367-1368,1369,1371-1372,1374-1375,1377-1378,1380-1381,1383-1384,1386-1387,1389-1390,1392-1393,1395-1396,1398-1399,1401-1402,1404-1405,1407-1408,1410-1411,1413-1414,1416-1417,1419-1420,1422-1423,1425-1426,1428-1429,1431-1432,1434-1435,1437-1438,1440-1441,1443-1444,1446-1447,1449-1450,1452-1453,1455-1456,1458-1459,1461-1462,1464-1465,1467-1468,1469,1471-1472,1474-1475,1477-1478,1480-1481,1483-1484,1486-1487,1489-1490,1492-1493,1495-1496,1498-1499,1501-1502,1504-1505,1507-1508,1510-1511,1513-1514,1516-1517,1519-1520,1522-1523,1525-1526,1528-1529,1531-1532,1534-1535,1537-1538,1540-1541,1543-1544,1546-1547,1549-1550,1552-1553,1555-1556,1558-1559,1561-1562,1564-1565,1567-1568,1569,1571-1572,1574-1575,1577-1578,1580-1581,1583-1584,1586-1587,1589-1590,1592-1593,1595-1596,1598-1599,1601-1602,1604-1605,1607-1608,1610-1611,1613-1614,1616-1617,1619-1620,1622-1623,1625-1626,1628-1629,1631-1632,1634-1635,1637-1638,1640-1641,1643-1644,1646-1647,1649-1650,1652-1653,1655-1656,1658-1659,1661-1662,1664-1665,1667-1668,1669,1671-1672,1674-1675,1677-1678,1680-1681,1683-1684,1686-1687,1689-1690,1692-1693,1695-1696,1698-1699,1701-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dvisc	0.0006283	Pa×s	466.27	Joback Method
dvisc	0.0003176	Pa×s	525.61	Joback Method
dvisc	0.0001844	Pa×s	584.94	Joback Method
dvisc	0.0001183	Pa×s	644.27	Joback Method
dvisc	0.0000818	Pa×s	703.61	Joback Method
dvisc	0.0000599	Pa×s	762.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349503&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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