

Heptadecafluorononanoic acid, octyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C17H17F17O2/c1-2-3-4-5-6-7-8-36-9(35)10(18,19)11(20,21)12(22,23)13(24,25)14(26,27)15(28,29)16(30,31)32(33,34)35(36,37)38(39,40)41(42,43)44(45,46)47(48,49)50(51,52)53(54,55)56(57,58)59(60,61)62(63,64)65(66,67)68(69,70)71(72,73)74(75,76)77(78,79)80(81,82)83(84,85)86(87,88)89(90,91)92(93,94)95(96,97)98(99,100)101(102,103)104(105,106)107(108,109)110(111,112)113(114,115)116(117,118)119(120,121)122(123,124)125(126,127)128(129,130)131(132,133)134(135,136)137(138,139)140(141,142)143(144,145)146(147,148)149(150,151)152(153,154)155(156,157)158(159,160)161(162,163)164(165,166)167(168,169)170(171,172)173(174,175)176(177,178)179(180,181)182(183,184)185(186,187)188(189,190)191(192,193)194(195,196)197(198,199)200(201,202)203(204,205)206(207,208)209(210,211)212(213,214)215(216,217)218(219,220)221(222,223)224(225,226)227(228,229)230(231,232)233(234,235)236(237,238)239(240,241)242(243,244)245(246,247)248(249,250)251(252,253)254(255,256)257(258,259)260(261,262)263(264,265)266(267,268)269(270,271)272(273,274)275(276,277)278(279,280)281(282,283)284(285,286)287(288,289)290(291,292)293(294,295)296(297,298)299(300,301)302(303,304)305(306,307)308(309,310)311(312,313)314(315,316)317(318,319)320(321,322)323(324,325)326(327,328)329(330,331)332(333,334)335(336,337)338(339,340)341(342,343)344(345,346)347(348,349)350(351,352)353(354,355)356(357,358)359(360,361)362(363,364)365(366,367)368(369,370)371(372,373)374(375,376)377(378,379)380(381,382)383(384,385)386(387,388)389(390,391)392(393,394)395(396,397)398(399,400)401(402,403)404(405,406)407(408,409)410(411,412)413(414,415)416(417,418)419(420,421)422(423,424)425(426,427)428(429,430)431(432,433)434(435,436)437(438,439)440(441,442)443(444,445)446(447,448)449(450,451)452(453,454)455(456,457)458(459,460)461(462,463)464(465,466)467(468,469)470(471,472)473(474,475)475(476,477)478(479,480)481(482,483)484(485,486)487(488,489)490(491,492)493(494,495)496(497,498)499(500,501)502(503,504)505(506,507)508(509,510)511(512,513)514(515,516)517(518,519)520(521,522)523(524,525)526(527,528)529(530,531)532(533,534)535(536,537)538(539,540)541(542,543)544(545,546)547(548,549)550(551,552)553(554,555)556(557,558)559(560,561)562(563,564)565(566,567)568(569,570)571(572,573)574(575,576)577(578,579)580(581,582)583(584,585)586(587,588)589(590,591)592(593,594)595(596,597)598(599,600)601(602,603)604(605,606)607(608,609)610(611,612)613(614,615)616(617,618)619(620,621)622(623,624)625(626,627)628(629,630)631(632,633)634(635,636)637(638,639)640(641,642)643(644,645)646(647,648)649(650,651)652(653,654)655(656,657)658(659,660)661(662,663)664(665,666)667(668,669)670(671,672)673(674,675)675(676,677)678(679,680)681(682,683)684(685,686)687(688,689)690(691,692)693(694,695)695(696,697)698(699,700)701(702,703)704(705,706)707(708,709)710(711,712)713(714,715)716(717,718)719(720,721)722(723,724)725(726,727)728(729,730)731(732,733)734(735,736)737(738,739)740(741,742)743(744,745)746(747,748)749(750,751)752(753,754)755(756,757)758(759,760)761(762,763)764(765,766)767(768,769)770(771,772)773(774,775)775(776,777)778(779,780)781(782,783)784(785,786)787(788,789)790(791,792)793(794,795)795(796,797)798(799,800)801(802,803)804(805,806)807(808,809)810(811,812)813(814,815)816(817,818)819(820,821)822(823,824)825(826,827)828(829,830)831(832,833)834(835,836)837(838,839)840(841,842)843(844,845)846(847,848)849(850,851)852(853,854)855(856,857)858(859,860)861(862,863)864(865,866)867(868,869)870(871,872)873(874,875)875(876,877)878(879,880)881(882,883)884(885,886)887(888,889)890(891,892)893(894,895)895(896,897)898(899,900)901(902,903)904(905,906)907(908,909)910(911,912)913(914,915)916(917,918)919(920,921)922(923,924)925(926,927)928(929,930)931(932,933)934(935,936)937(938,939)940(941,942)943(944,945)946(947,948)949(950,951)952(953,954)955(956,957)958(959,960)961(962,963)964(965,966)967(968,969)970(971,972)973(974,975)975(976,977)978(979,980)981(982,983)984(985,986)987(988,989)990(991,992)993(994,995)995(996,997)998(999,1000)1001(1002,1003)1004(1005,1006)1007(1008,1009)1010(1011,1012)1013(1014,1015)1016(1017,1018)1019(1020,1021)1022(1023,1024)1025(1026,1027)1028(1029,1030)1031(1032,1033)1034(1035,1036)1037(1038,1039)1040(1041,1042)1043(1044,1045)1046(1047,1048)1049(1050,1051)1052(1053,1054)1055(1056,1057)1058(1059,1060)1061(1062,1063)1064(1065,1066)1067(1068,1069)1070(1071,1072)1073(1074,1075)1075(1076,1077)1078(1079,1080)1081(1082,1083)1084(1085,1086)1087(1088,1089)1090(1091,1092)1093(1094,1095)1095(1096,1097)1098(1099,1100)1101(1102,1103)1104(1105,1106)1107(1108,1109)1110(1111,1112)1113(1114,1115)1116(1117,1118)1119(1120,1121)1122(1123,1124)1125(1126,1127)1128(1129,1130)1131(1132,1133)1134(1135,1136)1137(1138,1139)1140(1141,1142)1143(1144,1145)1146(1147,1148)1149(1150,1151)1152(1153,1154)1155(1156,1157)1158(1159,1160)1161(1162,1163)1164(1165,1166)1167(1168,1169)1170(1171,1172)1173(1174,1175)1175(1176,1177)1178(1179,1180)1181(1182,1183)1184(1185,1186)1187(1188,1189)1190(1191,1192)1193(1194,1195)1195(1196,1197)1198(1199,1200)1201(1202,1203)1204(1205,1206)1207(1208,1209)1210(1211,1212)1213(1214,1215)1216(1217,1218)1219(1220,1221)1222(1223,1224)1225(1226,1227)1228(1229,1230)1231(1232,1233)1234(1235,1236)1237(1238,1239)1240(1241,1242)1243(1244,1245)1246(1247,1248)1249(1250,1251)1252(1253,1254)1255(1256,1257)1258(1259,1260)1261(1262,1263)1264(1265,1266)1267(1268,1269)1270(1271,1272)1273(1274,1275)1275(1276,1277)1278(1279,1280)1281(1282,1283)1284(1285,1286)1287(1288,1289)1290(1291,1292)1293(1294,1295)1295(1296,1297)1298(1299,1300)1301(1302,1303)1304(1305,1306)1307(1308,1309)1310(1311,1312)1313(1314,1315)1316(1317,1318)1319(1320,1321)1322(1323,1324)1325(1326,1327)1328(1329,1330)1331(1332,1333)1334(1335,1336)1337(1338,1339)1340(1341,1342)1343(1344,1345)1346(1347,1348)1349(1350,1351)1352(1353,1354)1355(1356,1357)1358(1359,1360)1361(1362,1363)1364(1365,1366)1367(1368,1369)1370(1371,1372)1373(1374,1375)1375(1376,1377)1378(1379,1380)1381(1382,1383)1384(1385,1386)1387(1388,1389)1390(1391,1392)1393(1394,1395)1395(1396,1397)1398(1399,1400)1401(1402,1403)1404(1405,1406)1407(1408,1409)1410(1411,1412)1413(1414,1415)1416(1417,1418)1419(1420,1421)1422(1423,1424)1425(1426,1427)1428(1429,1430)1431(1432,1433)1434(1435,1436)1437(1438,1439)1440(1441,1442)1443(1444,1445)1446(1447,1448)1449(1450,1451)1452(1453,1454)1455(1456,1457)1458(1459,1460)1461(1462,1463)1464(1465,1466)1467(1468,1469)1470(1471,1472)1473(1474,1475)1475(1476,1477)1478(1479,1480)1481(1482,1483)1484(1485,1486)1487(1488,1489)1490(1491,1492)1493(1494,1495)1495(1496,1497)1498(1499,1500)1501(1502,1503)1504(1505,1506)1507(1508,1509)1510(1511,1512)1513(1514,1515)1516(1517,1518)1519(1520,1521)1522(1523,1524)1525(1526,1527)1528(1529,1530)1531(1532,1533)1534(1535,1536)1537(1538,1539)1540(1541,1542)1543(1544,1545)1546(1547,1548)1549(1550,1551)1552(1553,1554)1555(1556,1557)1558(1559,1560)1561(1562,1563)1564(1565,1566)1567(1568,1569)1570(1571,1572)1573(1574,1575)1575(1576,1577)1578(1579,1580)1581(1582,1583)1584(1585,1586)1587(1588,1589)1590(1591,1592)1593(1594,1595)1595(1596,1597)1598(1599,1600)1601(1602,1603)1604(1605,1606)1607(1608,1609)1610(1611,1612)1613(1614,1615)1616(1617,1618)1619(1620,1621)1622(1623,1624)1625(1626,1627)1628(1629,1630)1631(1632,1633)1634(1635,1636)1637(1638,1639)1640(1641,1642)1643(1644,1645)1646(1647,1648)1649(1650,1651)1652(1653,1654)1655(1656,1657)1658(1659,1660)1661(1662,1663)1664(1665,1666)1667(1668,1669)1670(1671,1672)1673(1674,1675)1675(1676,1677)1678(1679,1680)1681(1682,1683)1684(1685,1686)1687(1688,1689)1690(1691,1692)1693(1694,1695)1695(1696,1697)1698(1699,1700)1701(1702,1703)1704(1705,1706)1707(1708,1709)1710(1711,1712)1713(1714,1715)1716(1717,1718)1719(1720,1721)1722(1723,1724)1725(1726,1727)1728(1729,1730)1731(1732,1733)1734(1735,1736)1737(1738,1739)1740(1741,1742)1743(1744,1745)1746(1747,1748)1749(1750,1751)1752(1753,1754)1755(1756,1757)1758(1759,1760)1761(1762,1763)1764(1765,1766)1767(1768,1769)1770(1771,1772)1773(1774,1775)1775(1776,1777)1778(1779,1780)1781(1782,1783)1784(1785,1786)1787(1788,1789)1790(1791,1792)1793(1794,1795)1795(1796,1797)1798(1799,1800)1801(1802,1803)1804(1805,1806)1807(1808,1809)1810(1811,1812)1813(1814,1815)1816(1817,1818)1819(1820,1821)1822(1823,1824)1825(1826,1827)1828(1829,1830)1831(1832,1833)1834(1835,1836)1837(1838,1839)1840(1841,1842)1843(1844,1845)1846(1847,1848)1849(1850,1851)1852(1853,1854)1855(1856,1857)1858(1859,1860)1861(1862,1863)1864(1865,1866)1867(1868,1869)1870(1871,1872)1873(1874,1875)1875(1876,1877)1878(1879,1880)1881(1882,1883)1884(1885,1886)1887(1888,1889)1890(1891,1892)1893(1894,1895)1895(1896,1897)1898(1899,1900)1901(1902,1903)1904(1905,1906)1907(1908,1909)1910(1911,1912)1913(1914,1915)1916(1917,1918)1919(1920,1921)1922(1923,1924)1925(1926,1927)1928(1929,1930)1931(1932,1933)1934(1935,1936)1937(1938,1939)1940(1941,1942)1943(1944,1945)1946(1947,1948)1949(1950,1951)1952(1953,1954)1955(1956,1957)1958(1959,1960)1961(1962,1963)1964(1965,1966)1967(1968,1969)1970(1971,1972)1973(1974,1975)1975(1976,1977)1978(1979,1980)1981(1982,1983)1984(1985,1986)1987(1988,1989)1990(1991,1992)1993(1994,1995)1995(1996,1997)1998(1999,2000)2001(2002,2003)2004(2005,2006)2007(2008,2009)2010(2011,2012)2013(2014,2015)2016(2017,2018)2019(2020,2021)2022(2023,2024)2025(2026,2027)2028(2029,2030)2031(2032,2033)2034(2035,2036)2037(2038,2039)2040(2041,2042)2043(2044,2045)2046(2047,2048)2049(2050,2051)2052(2053,2054)2055(2056,2057)2058(2059,2060)2061(2062,2063)2064(2065,2066)2067(2068,2069)2070(2071,2072)2073(2074,2075)2075(2076,2077)2078(2079,2080)2081(2082,2083)2084(2085,2086)2087(2088,2089)2090(2091,2092)2093(2094,2095)2095(2096,2097)2098(2099,2100)2101(2102,2103)2104(2105,2106)2107(2108,2109)2110(2111,2112)2113(2114,2115)2116(2117,2118)2119(2120,2121)2122(2123,2124)2125(2126,2127)2128(2129,2130)2131(2132,2133)2134(2135,2136)2137(2138,2139)2140(2141,2142)2143(2144,2145)2146(2147,2148)2149(2150,2151)2152(2153,2154)2155(2156,2157)2158(2159,2160)2161(2162,2163)2164(2165,2166)2167(2168,2169)2170(2171,2172)2173(2174,2175)2175(2176,2177)2178(2179,2180)2181(2182,2183)2184(2185,2186)2187(2188,2189)2190(2191,2192)2193(2194,2195)2195(2196,2197)2198(2199,2200)2201(2202,2203)2204(2205,2206)2207(2208,2209)2210(2211,2212)2213(2214,2215)2216(2217,2218)2219(2220,2221)2222(2223,2224)2225(2226,2227)2228(2229,2230)2231(2232,2233)2234(2235,2236)2237(2238,2239)2240(2241,2242)2243(2244,2245)2246(2247,2248)2249(2250,2251)2252(2253,2254)2255(2256,2257)2258(2259,2260)2261(2262,2263)2264(2265,2266)2267(2268,2269)2270(2271,2272)2273(2274,2275)2275(2276,2277)2278(2279,2280)2281(2282,2283)2284(2285,2286)2287(2288,2289)2290(2291,2292)2293(2294,2295)2295(2296,2297)2298(2299,2300)2301(2302,2303)2304(2305,2306)2307(2308,2309)2310(2311,2312)2313(2314,2315)2316(2317,2318)2319(2320,2321)2322(2323,2324)2325(2326,2327)2328(2329,2330)2331(2332,2333)2334(2335,2336)2337(2338,2339)2340(2341,2342)2343(2344,2345)2346(2347,2348)2349(2350,2351)2352(2353,2354)2355(2356,2357)2358(2359,2360)2361(2362,2363)2364(2365,2366)2367(2368,2369)2370(2371,2372)2373(2374,2375)2375(2376,2377)2378(2379,2380)2381(2382,2383)2384(2385,2386)2387(2388,2389)2390(2391,2392)2393(2394,2395)2395(2396,2397)2398(2399,2400)2401(2402,2403)2404(2405,2406)2407(2408,2409)2410(2411,2412)2413(2414,2415)2416(2417,2418)2419(2420,2421)2422(2423,2424)2425(2426,2427)2428(2429,2430)2431(2432,2433)2434(2435,2436)2437(2438,2439)2440(2441,2442)2443(2444,2445)2446(2447,2448)2449(2450,2451)2452(2453,2454)2455(2456,2457)2458(2459,2460)2461(2462,2463)2464(2465,2466)2467(2468,2469)2470(2471,2472)2473(2474,2475)2475(2476,2477)2478(2479,2480)2481(2482,2483)2484(2485,2486)2487(2488,2489)2490(2491,2492)2493(2494,2495)2495(2496,2497)2498(2499,2500)2501(2502,2503)2504(2505,2506)2507(2508,2509)2510(2511,2512)2513(2514,2515)2516(2517,2518)2519(2520,2521)2522(2523,2524)2525(2526,2527)2528(2529,2530)2531(2532,2533)2534(2535,2536)2537(2538,2539)2540(2541,2542)2543(2544,2545)2546(2547,2548)2549(2550,2551)2552(2553,2554)2555(2556,2557)2558(2559,2560)2561(2562,2563)2564(2565,2566)2567(2568,2569)2570(2571,2572)2573(2574,2575)2575(2576,2577)2578(2579,2580)2581(2582,2583)2584(2585,2586)2587(2588,2589)2590(2591,2592)2593(2594,2595)2595(2596,2597)2598(2599,2600)2601(2602,2603)2604(2605,2606)2607(2608,2609)2610(2611,2612)2613(2614,2615)2616(2617,2618)2619(2620,2621)2622(2623,2624)2625(2626,2627)2628(2629,2630)263

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356024&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.chemeo.com/cid/44-114-6/Heptadecafluorononanoic-acid-octyl-ester.pdf>

Generated by Cheméo on 2024-04-24 07:21:20.575092658 +0000 UTC m=+16232529.495669974.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.