

Pentadecafluorooctanoic acid, dodecyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C20H25F15O2/c1-2-3-4-5-6-7-8-9-10-11-12-37-13(36)14(21,22)15(23,24)16(25,26)17(27,28)18(29,30)19(31,32)33(34,35)36(37,38)39(39,40)41(41,42)42(43,44)45(45,46)46(47,48)49(49,50)51(51,52)52(53,54)55(55,56)56(57,58)59(59,60)60(61,62)63(63,64)64(65,66)67(67,68)69(69,70)71(71,72)72(73,74)75(75,76)76(77,78)79(79,80)80(81,82)83(83,84)84(85,86)87(87,88)89(89,90)91(91,92)92(93,94)95(95,96)97(97,98)99(99,100)101(101,102)103(103,104)105(105,106)107(107,108)109(109,110)111(111,112)113(113,114)115(115,116)117(117,118)119(119,120)121(121,122)123(123,124)125(125,126)127(127,128)129(129,130)131(131,132)133(133,134)135(135,136)137(137,138)139(139,140)141(141,142)143(143,144)145(145,146)147(147,148)149(149,150)151(151,152)153(153,154)155(155,156)157(157,158)159(159,160)161(161,162)163(163,164)165(165,166)167(167,168)169(169,170)171(171,172)173(173,174)175(175,176)177(177,178)179(179,180)181(181,182)183(183,184)185(185,186)187(187,188)189(189,190)191(191,192)193(193,194)195(195,196)197(197,198)199(199,200)201(201,202)203(203,204)205(205,206)207(207,208)209(209,210)211(211,212)213(213,214)215(215,216)217(217,218)219(219,220)221(221,222)223(223,224)225(225,226)227(227,228)229(229,230)231(231,232)233(233,234)235(235,236)237(237,238)239(239,240)241(241,242)243(243,244)245(245,246)247(247,248)249(249,250)251(251,252)253(253,254)255(255,256)257(257,258)259(259,260)261(261,262)263(263,264)265(265,266)267(267,268)269(269,270)271(271,272)273(273,274)275(275,276)277(277,278)279(279,280)281(281,282)283(283,284)285(285,286)287(287,288)289(289,290)291(291,292)293(293,294)295(295,296)297(297,298)299(299,300)301(301,302)303(303,304)305(305,306)307(307,308)309(309,310)311(311,312)313(313,314)315(315,316)317(317,318)319(319,320)321(321,322)323(323,324)325(325,326)327(327,328)329(329,330)331(331,332)333(333,334)335(335,336)337(337,338)339(339,340)341(341,342)343(343,344)345(345,346)347(347,348)349(349,350)351(351,352)353(353,354)355(355,356)357(357,358)359(359,360)361(361,362)363(363,364)365(365,366)367(367,368)369(369,370)371(371,372)373(373,374)375(375,376)377(377,378)379(379,380)381(381,382)383(383,384)385(385,386)387(387,388)389(389,390)391(391,392)393(393,394)395(395,396)397(397,398)399(399,400)401(401,402)403(403,404)405(405,406)407(407,408)409(409,410)411(411,412)413(413,414)415(415,416)417(417,418)419(419,420)421(421,422)423(423,424)425(425,426)427(427,428)429(429,430)431(431,432)433(433,434)435(435,436)437(437,438)439(439,440)441(441,442)443(443,444)445(445,446)447(447,448)449(449,450)451(451,452)453(453,454)455(455,456)457(457,458)459(459,460)461(461,462)463(463,464)465(465,466)467(467,468)469(469,470)471(471,472)473(473,474)475(475,476)477(477,478)479(479,480)481(481,482)483(483,484)485(485,486)487(487,488)489(489,490)491(491,492)493(493,494)495(495,496)497(497,498)499(499,500)501(501,502)503(503,504)505(505,506)507(507,508)509(509,510)511(511,512)513(513,514)515(515,516)517(517,518)519(519,520)521(521,522)523(523,524)525(525,526)527(527,528)529(529,530)531(531,532)533(533,534)535(535,536)537(537,538)539(539,540)541(541,542)543(543,544)545(545,546)547(547,548)549(549,550)551(551,552)553(553,554)555(555,556)557(557,558)559(559,560)561(561,562)563(563,564)565(565,566)567(567,568)569(569,570)571(571,572)573(573,574)575(575,576)577(577,578)579(579,580)581(581,582)583(583,584)585(585,586)587(587,588)589(589,590)591(591,592)593(593,594)595(595,596)597(597,598)599(599,600)601(601,602)603(603,604)605(605,606)607(607,608)609(609,610)611(611,612)613(613,614)615(615,616)617(617,618)619(619,620)621(621,622)623(623,624)625(625,626)627(627,628)629(629,630)631(631,632)633(633,634)635(635,636)637(637,638)639(639,640)641(641,642)643(643,644)645(645,646)647(647,648)649(649,650)651(651,652)653(653,654)655(655,656)657(657,658)659(659,660)661(661,662)663(663,664)665(665,666)667(667,668)669(669,670)671(671,672)673(673,674)675(675,676)677(677,678)679(679,680)681(681,682)683(683,684)685(685,686)687(687,688)689(689,690)691(691,692)693(693,694)695(695,696)697(697,698)699(699,700)701(701,702)703(703,704)705(705,706)707(707,708)709(709,710)711(711,712)713(713,714)715(715,716)717(717,718)719(719,720)721(721,722)723(723,724)725(725,726)727(727,728)729(729,730)731(731,732)733(733,734)735(735,736)737(737,738)739(739,740)741(741,742)743(743,744)745(745,746)747(747,748)749(749,750)751(751,752)753(753,754)755(755,756)757(757,758)759(759,760)761(761,762)763(763,764)765(765,766)767(767,768)769(769,770)771(771,772)773(773,774)775(775,776)777(777,778)779(779,780)781(781,782)783(783,784)785(785,786)787(787,788)789(789,790)791(791,792)793(793,794)795(795,796)797(797,798)799(799,800)801(801,802)803(803,804)805(805,806)807(807,808)809(809,810)811(811,812)813(813,814)815(815,816)817(817,818)819(819,820)821(821,822)823(823,824)825(825,826)827(827,828)829(829,830)831(831,832)833(833,834)835(835,836)837(837,838)839(839,840)841(841,842)843(843,844)845(845,846)847(847,848)849(849,850)851(851,852)853(853,854)855(855,856)857(857,858)859(859,860)861(861,862)863(863,864)865(865,866)867(867,868)869(869,870)871(871,872)873(873,874)875(875,876)877(877,878)879(879,880)881(881,882)883(883,884)885(885,886)887(887,888)889(889,890)891(891,892)893(893,894)895(895,896)897(897,898)899(899,900)901(901,902)903(903,904)905(905,906)907(907,908)909(909,910)911(911,912)913(913,914)915(915,916)917(917,918)919(919,920)921(921,922)923(923,924)925(925,926)927(927,928)929(929,930)931(931,932)933(933,934)935(935,936)937(937,938)939(939,940)941(941,942)943(943,944)945(945,946)947(947,948)949(949,950)951(951,952)953(953,954)955(955,956)957(957,958)959(959,960)961(961,962)963(963,964)965(965,966)967(967,968)969(969,970)971(971,972)973(973,974)975(975,976)977(977,978)979(979,980)981(981,982)983(983,984)985(985,986)987(987,988)989(989,990)991(991,992)993(993,994)995(995,996)997(997,998)999(999,1000)1001(1001,1002)1003(1003,1004)1005(1005,1006)1007(1007,1008)1009(1009,1010)1011(1011,1012)1013(1013,1014)1015(1015,1016)1017(1017,1018)1019(1019,1020)1021(1021,1022)1023(1023,1024)1025(1025,1026)1027(1027,1028)1029(1029,1030)1031(1031,1032)1033(1033,1034)1035(1035,1036)1037(1037,1038)1039(1039,1040)1041(1041,1042)1043(1043,1044)1045(1045,1046)1047(1047,1048)1049(1049,1050)1051(1051,1052)1053(1053,1054)1055(1055,1056)1057(1057,1058)1059(1059,1060)1061(1061,1062)1063(1063,1064)1065(1065,1066)1067(1067,1068)1069(1069,1070)1071(1071,1072)1073(1073,1074)1075(1075,1076)1077(1077,1078)1079(1079,1080)1081(1081,1082)1083(1083,1084)1085(1085,1086)1087(1087,1088)1089(1089,1090)1091(1091,1092)1093(1093,1094)1095(1095,1096)1097(1097,1098)1099(1099,1100)1101(1101,1102)1103(1103,1104)1105(1105,1106)1107(1107,1108)1109(1109,1110)1111(1111,1112)1113(1113,1114)1115(1115,1116)1117(1117,1118)1119(1119,1120)1121(1121,1122)1123(1123,1124)1125(1125,1126)1127(1127,1128)1129(1129,1130)1131(1131,1132)1133(1133,1134)1135(1135,1136)1137(1137,1138)1139(1139,1140)1141(1141,1142)1143(1143,1144)1145(1145,1146)1147(1147,1148)1149(1149,1150)1151(1151,1152)1153(1153,1154)1155(1155,1156)1157(1157,1158)1159(1159,1160)1161(1161,1162)1163(1163,1164)1165(1165,1166)1167(1167,1168)1169(1169,1170)1171(1171,1172)1173(1173,1174)1175(1175,1176)1177(1177,1178)1179(1179,1180)1181(1181,1182)1183(1183,1184)1185(1185,1186)1187(1187,1188)1189(1189,1190)1191(1191,1192)1193(1193,1194)1195(1195,1196)1197(1197,1198)1199(1199,1200)1201(1201,1202)1203(1203,1204)1205(1205,1206)1207(1207,1208)1209(1209,1210)1211(1211,1212)1213(1213,1214)1215(1215,1216)1217(1217,1218)1219(1219,1220)1221(1221,1222)1223(1223,1224)1225(1225,1226)1227(1227,1228)1229(1229,1230)1231(1231,1232)1233(1233,1234)1235(1235,1236)1237(1237,1238)1239(1239,1240)1241(1241,1242)1243(1243,1244)1245(1245,1246)1247(1247,1248)1249(1249,1250)1251(1251,1252)1253(1253,1254)1255(1255,1256)1257(1257,1258)1259(1259,1260)1261(1261,1262)1263(1263,1264)1265(1265,1266)1267(1267,1268)1269(1269,1270)1271(1271,1272)1273(1273,1274)1275(1275,1276)1277(1277,1278)1279(1279,1280)1281(1281,1282)1283(1283,1284)1285(1285,1286)1287(1287,1288)1289(1289,1290)1291(1291,1292)1293(1293,1294)1295(1295,1296)1297(1297,1298)1299(1299,1300)1301(1301,1302)1303(1303,1304)1305(1305,1306)1307(1307,1308)1309(1309,1310)1311(1311,1312)1313(1313,1314)1315(1315,1316)1317(1317,1318)1319(1319,1320)1321(1321,1322)1323(1323,1324)1325(1325,1326)1327(1327,1328)1329(1329,1330)1331(1331,1332)1333(1333,1334)1335(1335,1336)1337(1337,1338)1339(1339,1340)1341(1341,1342)1343(1343,1344)1345(1345,1346)1347(1347,1348)1349(1349,1350)1351(1351,1352)1353(1353,1354)1355(1355,1356)1357(1357,1358)1359(1359,1360)1361(1361,1362)1363(1363,1364)1365(1365,1366)1367(1367,1368)1369(1369,1370)1371(1371,1372)1373(1373,1374)1375(1375,1376)1377(1377,1378)1379(1379,1380)1381(1381,1382)1383(1383,1384)1385(1385,1386)1387(1387,1388)1389(1389,1390)1391(1391,1392)1393(1393,1394)1395(1395,1396)1397(1397,1398)1399(1399,1400)1401(1401,1402)1403(1403,1404)1405(1405,1406)1407(1407,1408)1409(1409,1410)1411(1411,1412)1413(1413,1414)1415(1415,1416)1417(1417,1418)1419(1419,1420)1421(1421,1422)1423(1423,1424)1425(1425,1426)1427(1427,1428)1429(1429,1430)1431(1431,1432)1433(1433,1434)1435(1435,1436)1437(1437,1438)1439(1439,1440)1441(1441,1442)1443(1443,1444)1445(1445,1446)1447(1447,1448)1449(1449,1450)1451(1451,1452)1453(1453,1454)1455(1455,1456)1457(1457,1458)1459(1459,1460)1461(1461,1462)1463(1463,1464)1465(1465,1466)1467(1467,1468)1469(1469,1470)1471(1471,1472)1473(1473,1474)1475(1475,1476)1477(1477,1478)1479(1479,1480)1481(1481,1482)1483(1483,1484)1485(1485,1486)1487(1487,1488)1489(1489,1490)1491(1491,1492)1493(1493,1494)1495(1495,1496)1497(1497,1498)1499(1499,1500)1501(1501,1502)1503(1503,1504)1505(1505,1506)1507(1507,1508)1509(1509,1510)1511(1511,1512)1513(1513,1514)1515(1515,1516)1517(1517,1518)1519(1519,1520)1521(1521,1522)1523(1523,1524)1525(1525,1526)1527(1527,1528)1529(1529,1530)1531(1531,1532)1533(1533,1534)1535(1535,1536)1537(1537,1538)1539(1539,1540)1541(1541,1542)1543(1543,1544)1545(1545,1546)1547(1547,1548)1549(1549,1550)1551(1551,1552)1553(1553,1554)1555(1555,1556)1557(1557,1558)1559(1559,1560)1561(1561,1562)1563(1563,1564)1565(1565,1566)1567(1567,1568)1569(1569,1570)1571(1571,1572)1573(1573,1574)1575(1575,1576)1577(1577,1578)1579(1579,1580)1581(1581,1582)1583(1583,1584)1585(1585,1586)1587(1587,1588)1589(1589,1590)1591(1591,1592)1593(1593,1594)1595(1595,1596)1597(1597,1598)1599(1599,1600)1601(1601,1602)1603(1603,1604)1605(1605,1606)1607(1607,1608)1609(1609,1610)1611(1611,1612)1613(1613,1614)1615(1615,1616)1617(1617,1618)1619(1619,1620)1621(1621,1622)1623(1623,1624)1625(1625,1626)1627(1627,1628)1629(1629,1630)1631(1631,1632)1633(1633,1634)1635(1635,1636)1637(1637,1638)1639(1639,1640)1641(1641,1642)1643(1643,1644)1645(1645,1646)1647(1647,1648)1649(1649,1650)1651(1651,1652)1653(1653,1654)1655(1655,1656)1657(1657,1658)1659(1659,1660)1661(1661,1662)1663(1663,1664)1665(1665,1666)1667(1667,1668)1669(1669,1670)1671(1671,1672)1673(1673,1674)1675(1675,1676)1677(1677,1678)1679(1679,1680)1681(1681,1682)1683(1683,1684)1685(1685,1686)1687(1687,1688)1689(1689,1690)1691(1691,1692)1693(1693,1694)1695(1695,1696)1697(1697,1698)1699(1699,1700)1701(1701,1702)1703(1703,1704)1705(1705,1706)1707(1707,1708)1709(1709,1710)1711(1711,1712)1713(1713,1714)1715(1715,1716)1717(1717,1718)1719(1719,1720)1721(1721,1722)1723(1723,1724)1725(1725,1726)1727(1727,1728)1729(1729,1730)1731(1731,1732)1733(1733,1734)1735(1735,1736)1737(1737,1738)1739(1739,1740)1741(1741,1742)1743(1743,1744)1745(1745,1746)1747(1747,1748)1749(1749,1750)1751(1751,1752)1753(1753,1754)1755(1755,1756)1757(1757,1758)1759(1759,1760)1761(1761,1762)1763(1763,1764)1765(1765,1766)1767(1767,1768)1769(1769,1770)1771(1771,1772)1773(1773,1774)1775(1775,1776)1777(1777,1778)1779(1779,1780)1781(1781,1782)1783(1783,1784)1785(1785,1786)1787(1787,1788)1789(1789,1790)1791(1791,1792)1793(1793,1794)1795(1795,1796)1797(1797,1798)1799(1799,1800)1801(1801,1802)1803(1803,1804)1805(1805,1806)1807(1807,1808)1809(1809,1810)1811(1811,1812)1813(1813,1814)1815(1815,1816)1817(1817,1818)1819(1819,1820)1821(1821,1822)1823(1823,1824)1825(1825,1826)1827(1827,1828)1829(1829,1830)1831(1831,1832)1833(1833,1834)1835(1835,1836)1837(1837,1838)1839(1839,1840)1841(1841,1842)1843(1843,1844)1845(1845,1846)1847(1847,1848)1849(1849,1850)1851(1851,1852)1853(1853,1854)1855(1855,1856)1857(1857,1858)1859(1859,1860)1861

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406042&Units=SI
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
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.cheméo.com/cid/72-649-2/Pentadecafluorooctanoic-acid-dodecyl-ester.pdf>

Generated by Cheméo on 2025-12-05 10:22:13.817101413 +0000 UTC m=+4678331.347142067.

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