

Heptadecafluorononanoic acid, decyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C19H21F17O2/c1-2-3-4-5-6-7-8-9-10-38-11(37)12(20,21)13(22,23)14(24,25)15(26,27)28(29,30)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)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)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(499,500)501(501,502)504(505,506)507(507,508)510(509,510)513(511,512)516(513,514)519(515,516)522(517,518)525(519,520)528(521,522)531(523,524)534(525,526)537(527,528)540(529,530)543(531,532)546(533,534)549(535,536)552(537,538)555(539,540)558(541,542)561(543,544)564(545,546)567(547,548)570(549,550)573(551,552)576(553,554)579(555,556)582(557,558)585(559,560)588(561,562)591(563,564)594(565,566)597(567,568)600(569,570)603(571,572)606(573,574)609(575,576)612(577,578)615(579,580)618(581,582)621(583,584)624(585,586)627(587,588)630(589,590)633(591,592)636(593,594)639(595,596)642(597,598)645(599,600)648(601,602)651(603,604)654(605,606)657(607,608)660(609,610)663(611,612)666(613,614)669(615,616)672(617,618)675(619,620)678(621,622)681(623,624)684(625,626)687(627,628)690(629,630)693(631,632)696(633,634)699(635,636)702(637,638)705(639,640)708(641,642)711(643,644)714(645,646)717(647,648)720(649,650)723(651,652)726(653,654)729(655,656)732(657,658)735(659,660)738(661,662)741(663,664)744(665,666)747(667,668)750(669,670)753(671,672)756(673,674)759(675,676)762(677,678)765(679,680)768(681,682)771(683,684)774(685,686)777(687,688)780(689,690)783(691,692)786(693,694)789(695,696)792(697,698)795(699,700)798(701,702)801(703,704)804(705,706)807(707,708)810(709,710)813(711,712)816(713,714)819(715,716)822(717,718)825(719,720)828(721,722)831(723,724)834(725,726)837(727,728)840(729,730)843(731,732)846(733,734)849(735,736)852(737,738)855(739,740)858(741,742)861(743,744)864(745,746)867(747,748)870(749,750)873(751,752)876(753,754)879(755,756)882(757,758)885(759,760)888(761,762)891(763,764)894(765,766)897(767,768)900(769,770)903(771,772)906(773,774)909(775,776)912(777,778)915(779,780)918(781,782)921(783,784)924(785,786)927(787,788)930(789,790)933(791,792)936(793,794)939(795,796)942(797,798)945(799,800)948(801,802)951(803,804)954(805,806)957(807,808)960(809,810)963(811,812)966(813,814)969(815,816)972(817,818)975(819,820)978(821,822)981(823,824)984(825,826)987(827,828)990(829,830)993(831,832)996(833,834)999(835,836)1002(837,838)1005(839,840)1008(841,842)1011(843,844)1014(845,846)1017(847,848)1020(849,850)1023(851,852)1026(853,854)1029(855,856)1032(857,858)1035(859,860)1038(861,862)1041(863,864)1044(865,866)1047(867,868)1050(869,870)1053(871,872)1056(873,874)1059(875,876)1062(877,878)1065(879,880)1068(881,882)1071(883,884)1074(885,886)1077(887,888)1080(889,890)1083(891,892)1086(893,894)1089(895,896)1092(897,898)1095(899,900)1098(901,902)1101(903,904)1104(905,906)1107(907,908)1110(909,910)1113(911,912)1116(913,914)1119(915,916)1122(917,918)1125(919,920)1128(921,922)1131(923,924)1134(925,926)1137(927,928)1140(929,930)1143(931,932)1146(933,934)1149(935,936)1152(937,938)1155(939,940)1158(941,942)1161(943,944)1164(945,946)1167(947,948)1170(949,950)1173(951,952)1176(953,954)1179(955,956)1182(957,958)1185(959,960)1188(961,962)1191(963,964)1194(965,966)1197(967,968)1200(969,970)1203(971,972)1206(973,974)1209(975,976)1212(977,978)1215(979,980)1218(981,982)1221(983,984)1224(985,986)1227(987,988)1230(989,990)1233(991,992)1236(993,994)1239(995,996)1242(997,998)1245(999,1000)1248(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Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356026&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvac:	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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