

Heptadecafluorononanoic acid, undecyl ester

Inchi:	InChI=1S/C20H23F17O2/c1-2-3-4-5-6-7-8-9-10-11-39-12(38)13(21,22)14(23,24)15(25,26)16(27,28)17(29,30)18(31,32)19(33,34)20(35,36)37(37,38)39(39,40)41(41,42)42(43,44)43(45,46)44(47,48)45(49,50)46(51,52)47(53,54)48(55,56)49(57,58)50(59,60)51(61,62)52(63,64)53(65,66)54(67,68)55(69,70)56(71,72)57(73,74)58(75,76)59(77,78)60(79,80)61(81,82)62(83,84)63(85,86)64(87,88)65(89,90)66(91,92)67(93,94)68(95,96)69(97,98)70(99,100)71(101,102)72(103,104)73(105,106)74(107,108)75(109,110)76(111,112)77(113,114)78(115,116)79(117,118)80(119,120)81(121,122)82(123,124)83(125,126)84(127,128)85(129,130)86(131,132)87(133,134)88(135,136)89(137,138)90(139,140)91(141,142)92(143,144)93(145,146)94(147,148)95(149,150)96(151,152)97(153,154)98(155,156)99(157,158)100(159,160)101(161,162)102(163,164)103(165,166)104(167,168)105(169,170)106(171,172)107(173,174)108(175,176)109(177,178)110(179,180)111(181,182)112(183,184)113(185,186)114(187,188)115(189,190)116(191,192)117(193,194)118(195,196)119(197,198)120(199,200)121(201,202)122(203,204)123(205,206)124(207,208)125(209,210)126(211,212)127(213,214)128(215,216)129(217,218)130(219,220)131(221,222)132(223,224)133(225,226)134(227,228)135(229,230)136(231,232)137(233,234)138(235,236)139(237,238)140(239,240)141(241,242)142(243,244)143(245,246)144(247,248)145(249,250)146(251,252)147(253,254)148(255,256)149(257,258)150(259,260)151(261,262)152(263,264)153(265,266)154(267,268)155(269,270)156(271,272)157(273,274)158(275,276)159(277,278)160(279,280)161(281,282)162(283,284)163(285,286)164(287,288)165(289,290)166(291,292)167(293,294)168(295,296)169(297,298)170(299,300)171(301,302)172(303,304)173(305,306)174(307,308)175(309,310)176(311,312)177(313,314)178(315,316)179(317,318)180(319,320)181(321,322)182(323,324)183(325,326)184(327,328)185(329,330)186(331,332)187(333,334)188(335,336)189(337,338)190(339,340)191(341,342)192(343,344)193(345,346)194(347,348)195(349,350)196(351,352)197(353,354)198(355,356)199(357,358)200(359,360)201(361,362)202(363,364)203(365,366)204(367,368)205(369,370)206(371,372)207(373,374)208(375,376)209(377,378)210(379,380)211(381,382)212(383,384)213(385,386)214(387,388)215(389,390)216(391,392)217(393,394)218(395,396)219(397,398)220(399,400)221(401,402)222(403,404)223(405,406)224(407,408)225(409,410)226(411,412)227(413,414)228(415,416)229(417,418)230(419,420)231(421,422)232(423,424)233(425,426)234(427,428)235(429,430)236(431,432)237(433,434)238(435,436)239(437,438)240(439,440)241(441,442)242(443,444)243(445,446)244(447,448)245(449,450)246(451,452)247(453,454)248(455,456)249(457,458)250(459,460)251(461,462)252(463,464)253(465,466)254(467,468)255(469,470)256(471,472)257(473,474)258(475,476)259(477,478)260(479,480)261(481,482)262(483,484)263(485,486)264(487,488)265(489,490)266(491,492)267(493,494)268(495,496)269(497,498)270(499,500)271(501,502)272(503,504)273(505,506)274(507,508)275(509,510)276(511,512)277(513,514)278(515,516)279(517,518)280(519,520)281(521,522)282(523,524)283(525,526)284(527,528)285(529,530)286(531,532)287(533,534)288(535,536)289(537,538)290(539,540)291(541,542)292(543,544)293(545,546)294(547,548)295(549,550)296(551,552)297(553,554)298(555,556)299(557,558)300(559,560)301(561,562)302(563,564)303(565,566)304(567,568)305(569,570)306(571,572)307(573,574)308(575,576)309(577,578)310(579,580)311(581,582)312(583,584)313(585,586)314(587,588)315(589,590)316(591,592)317(593,594)318(595,596)319(597,598)320(599,600)321(601,602)322(603,604)323(605,606)324(607,608)325(609,610)326(611,612)327(613,614)328(615,616)329(617,618)330(619,620)331(621,622)332(623,624)333(625,626)334(627,628)335(629,630)336(631,632)337(633,634)338(635,636)339(637,638)340(639,640)341(641,642)342(643,644)343(645,646)344(647,648)345(649,650)346(651,652)347(653,654)348(655,656)349(657,658)350(659,660)351(661,662)352(663,664)353(665,666)354(667,668)355(669,670)356(671,672)357(673,674)358(675,676)359(677,678)360(679,680)361(681,682)362(683,684)363(685,686)364(687,688)365(689,690)366(691,692)367(693,694)368(695,696)369(697,698)370(699,700)371(701,702)372(703,704)373(705,706)374(707,708)375(709,710)376(711,712)377(713,714)378(715,716)37
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Physical Properties

Property code	Value	Unit	Source
gf	-3405.45	kJ/mol	Joback Method
hf	-4104.80	kJ/mol	Joback Method
hfus	43.39	kJ/mol	Joback Method
hvap	45.01	kJ/mol	Joback Method
log10ws	-9.92		Crippen Method
logp	9.070		Crippen Method
mcvol	330.190	ml/mol	McGowan Method
pc	728.49	kPa	Joback Method
rinpol	1586.00		NIST Webbook
tb	695.04	K	Joback Method
tc	851.25	K	Joback Method
tf	416.71	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.83	J/mol×K	695.04	Joback Method
cpg	1069.68	J/mol×K	721.08	Joback Method
cpg	1084.46	J/mol×K	747.11	Joback Method
cpg	1098.27	J/mol×K	773.15	Joback Method
cpg	1111.19	J/mol×K	799.18	Joback Method
cpg	1123.31	J/mol×K	825.22	Joback Method
cpg	1134.71	J/mol×K	851.25	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U356027&Units=SI

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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