

Methyl perfluoroundecanoate

Inchi: InChI=1S/C12H3F21O2/c1-35-2(34)3(13,14)4(15,16)5(17,18)6(19,20)7(21,22)8(23,24)9(25,26)10(27,28)11(29,30)12(31,32)33(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(89,90)91(91,92)93(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)8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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=R385976&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
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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