

Perfluorododecane

Other names:	dodecane, hexacosafuoro- hexacosafuorododecane n-Perfluorododecane
Inchi:	InChI=1S/C12F26/c13-1(14,3(17,18)5(21,22)7(25,26)9(29,30)11(33,34)35)2(15,16)4(19,20)6(23,24)8(27,28)10(31,32)12(36,37)16(41,42)18(45,46)20(49,50)22(53,54)24(57,58)26(61,62)28(65,66)30(69,70)32(73,74)34(77,78)36(81,82)38(85,86)40(89,90)42(93,94)44(97,98)46(101,102)48(105,106)50(109,110)52(113,114)54(117,118)56(121,122)58(125,126)60(129,130)62(133,134)64(137,138)66(141,142)68(145,146)70(149,150)72(153,154)74(157,158)76(161,162)78(165,166)80(169,170)82(173,174)84(177,178)86(181,182)88(185,186)90(189,190)92(193,194)94(197,198)96(201,202)98(205,206)100(209,210)102(213,214)104(217,218)106(221,222)108(225,226)110(229,230)112(233,234)114(237,238)116(241,242)118(245,246)120(249,250)122(253,254)124(257,258)126(261,262)128(265,266)130(269,270)132(273,274)134(277,278)136(281,282)138(285,286)140(289,290)142(293,294)144(297,298)146(301,302)148(305,306)150(309,310)152(313,314)154(317,318)156(321,322)158(325,326)160(329,330)162(333,334)164(337,338)166(341,342)168(345,346)170(349,350)172(353,354)174(357,358)176(361,362)178(365,366)180(369,370)182(373,374)184(377,378)186(381,382)188(385,386)190(389,390)192(393,394)194(397,398)196(401,402)198(405,406)200(409,410)202(413,414)204(417,418)206(421,422)208(425,426)210(429,430)212(433,434)214(437,438)216(441,442)218(445,446)220(449,450)222(453,454)224(457,458)226(461,462)228(465,466)230(469,470)232(473,474)234(477,478)236(481,482)238(485,486)240(489,490)242(493,494)244(497,498)246(501,502)248(505,506)250(509,510)252(513,514)254(517,518)256(521,522)258(525,526)260(529,530)262(533,534)264(537,538)266(541,542)268(545,546)270(549,550)272(553,554)274(557,558)276(561,562)278(565,566)280(569,570)282(573,574)284(577,578)286(581,582)288(585,586)290(589,590)292(593,594)294(597,598)296(601,602)298(605,606)300(609,610)302(613,614)304(617,618)306(621,622)308(625,626)310(629,630)312(633,634)314(637,638)316(641,642)318(645,646)320(649,650)322(653,654)324(657,658)326(661,662)328(665,666)330(669,670)332(673,674)334(677,678)336(681,682)338(685,686)340(689,690)342(693,694)344(697,698)346(701,702)348(705,706)350(709,710)352(713,714)354(717,718)356(721,722)358(725,726)360(729,730)362(733,734)364(737,738)366(741,742)368(745,746)370(749,750)372(753,754)374(757,758)376(761,762)378(765,766)380(769,770)382(773,774)384(777,778)386(781,782)388(785,786)390(789,790)392(793,794)394(797,798)396(801,802)398(805,806)400(809,810)402(813,814)404(817,818)406(821,822)408(825,826)410(829,830)412(833,834)414(837,838)416(841,842)418(845,846)420(849,850)422(853,854)424(857,858)426(861,862)428(865,866)430(869,870)432(873,874)434(877,878)436(881,882)438(885,886)440(889,890)442(893,894)444(897,898)446(901,902)448(905,906)450(909,910)452(913,914)454(917,918)456(921,922)458(925,926)460(929,930)462(933,934)464(937,938)466(941,942)468(945,946)470(949,950)472(953,954)474(957,958)476(961,962)478(965,966)480(969,970)482(973,974)484(977,978)486(981,982)488(985,986)490(989,990)492(993,994)494(997,998)496(1001,1002)498(1005,1006)500(1009,1010)502(1013,1014)504(1017,1018)506(1021,1022)508(1025,1026)510(1029,1030)512(1033,1034)514(1037,1038)516(1041,1042)518(1045,1046)520(1049,1050)522(1053,1054)524(1057,1058)526(1061,1062)528(1065,1066)530(1069,1070)532(1073,1074)534(1077,1078)536(1081,1082)538(1085,1086)540(1089,1090)542(1093,1094)544(1097,1098)546(1101,1102)548(1105,1106)550(1109,1110)552(1113,1114)554(1117,1118)556(1121,1122)558(1125,1126)560(1129,1130)562(1133,1134)564(1137,1138)566(1141,1142)568(1145,1146)570(1149,1150)572(1153,1154)574(1157,1158)576(1161,1162)578(1165,1166)580(1169,1170)582(1173,1174)584(1177,1178)586(1181,1182)588(1185,1186)590(1189,1190)592(1193,1194)594(1197,1198)596(1201,1202)598(1205,1206)600(1209,1210)602(1213,1214)604(1217,1218)606(1221,1222)608(1225,1226)610(1229,1230)612(1233,1234)614(1237,1238)616(1241,1242)618(1245,1246)620(1249,1250)622(1253,1254)624(1257,1258)626(1261,1262)628(1265,1266)630(1269,1270)632(1273,1274)634(1277,1278)636(1281,1282)638(1285,1286)640(1289,1290)642(1293,1294)644(1297,1298)646(1301,1302)648(1305,1306)650(1309,1310)652(1313,1314

Physical Properties

Property code	Value	Unit	Source
gf	-4980.82	kJ/mol	Joback Method
hf	-5494.87	kJ/mol	Joback Method
hfus	24.20	kJ/mol	Applications of Correlation Gas Chromatography and Transpiration Studies for the Evaluation of the Vaporization and Sublimation Enthalpies of Some Perfluorinated Hydrocarbons
hvap	5.51	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	8.464		Crippen Method
mcvol	225.960	ml/mol	McGowan Method
pc	911.63	kPa	Joback Method
rinpol	528.00		NIST Webbook
rinpol	528.00		NIST Webbook
ss	763.30	J/mol×K	NIST Webbook
tb	416.22	K	Joback Method
tc	517.74	K	Joback Method
tf	348.50 ± 0.50	K	NIST Webbook
tf	348.00 ± 0.10	K	NIST Webbook
tf	347.60 ± 0.20	K	NIST Webbook
tf	348.20 ± 0.20	K	NIST Webbook
tf	347.30 ± 0.20	K	NIST Webbook
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.98	J/mol×K	416.22	Joback Method
cpg	700.59	J/mol×K	500.82	Joback Method
cpg	688.41	J/mol×K	483.90	Joback Method
cpg	675.39	J/mol×K	466.98	Joback Method
cpg	661.50	J/mol×K	450.06	Joback Method
cpg	646.71	J/mol×K	433.14	Joback Method
cpg	711.97	J/mol×K	517.74	Joback Method
cps	546.80	J/mol×K	298.15	NIST Webbook
hfust	38.16	kJ/mol	348.50	NIST Webbook
hfust	6.90	kJ/mol	170.20	NIST Webbook
hfust	38.16	kJ/mol	348.50	NIST Webbook
sfust	109.50	J/mol×K	348.50	NIST Webbook
sfust	40.54	J/mol×K	170.20	NIST Webbook

Sources

Applications of Correlation Gas Chromatography and Transpiration Sources for the Evaluation of the Vaporization and Sublimation Enthalpies of Some Perfluorinated Hydrocarbons:
NIST Webbook:

<https://www.doi.org/10.1021/je300504f>

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C307595&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
cps: Solid phase heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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