

# Perfluoroeicosane

|                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
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| <b>Other names:</b> | dotetracontafluoroeicosane<br>dotetracontafluoroicosane<br>eicosane, dotetracontafluoro-                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| <b>Inchi:</b>       | InChI=1S/C20F42/c21-1(22,3(25,26)5(29,30)7(33,34)9(37,38)11(41,42)13(45,46)15(49,50)17(53,54)19(57,58)23(61,62)25(65,66)27(69,70)29(73,74)31(77,78)33(81,82)35(85,86)37(89,90)39(93,94)41(97,98)43(101,102)45(105,106)47(109,110)49(113,114)51(117,118)53(121,122)55(125,126)57(129,130)59(133,134)61(137,138)63(141,142)65(145,146)67(149,150)69(153,154)71(157,158)73(161,162)75(165,166)77(169,170)79(173,174)81(177,178)83(181,182)85(185,186)87(189,190)89(193,194)91(197,198)93(201,202)95(205,206)97(209,210)99(213,214)101(217,218)103(221,222)105(225,226)107(229,230)109(233,234)111(237,238)113(241,242)115(245,246)117(249,250)119(253,254)121(257,258)123(261,262)125(265,266)127(269,270)129(273,274)131(277,278)133(281,282)135(285,286)137(289,290)139(293,294)141(297,298)143(301,302)145(305,306)147(309,310)149(313,314)151(317,318)153(321,322)155(325,326)157(329,330)159(333,334)161(337,338)163(341,342)165(345,346)167(349,350)169(353,354)171(357,358)173(361,362)175(365,366)177(369,370)179(373,374)181(377,378)183(381,382)185(385,386)187(389,390)189(393,394)191(397,398)193(401,402)195(405,406)197(409,410)199(413,414)201(417,418)203(421,422)205(425,426)207(429,430)209(433,434)211(437,438)213(441,442)215(445,446)217(449,450)219(453,454)221(457,458)223(461,462)225(465,466)227(469,470)229(473,474)231(477,478)233(481,482)235(485,486)237(489,490)239(493,494)241(497,498)243(501,502)245(505,506)247(509,510)249(513,514)251(517,518)253(521,522)255(525,526)257(529,530)259(533,534)261(537,538)263(541,542)265(545,546)267(549,550)269(553,554)271(557,558)273(561,562)275(565,566)277(569,570)279(573,574)281(577,578)283(581,582)285(585,586)287(589,590)289(593,594)291(597,598)293(601,602)295(605,606)297(609,610)299(613,614)301(617,618)303(621,622)305(625,626)307(629,630)309(633,634)311(637,638)313(641,642)315(645,646)317(649,650)319(653,654)321(657,658)323(661,662)325(665,666)327(669,670)329(673,674)331(677,678)333(681,682)335(685,686)337(689,690)339(693,694)341(697,698)343(701,702)345(705,706)347(709,710)349(713,714)351(717,718)353(721,722)355(725,726)357(729,730)359(733,734)361(737,738)363(741,742)365(745,746)367(749,750)369(753,754)371(757,758)373(761,762)375(765,766)377(769,770)379(773,774)381(777,778)383(781,782)385(785,786)387(789,790)389(793,794)391(797,798)393(801,802)395(805,806)397(809,810)399(813,814)401(817,818)403(821,822)405(825,826)407(829,830)409(833,834)411(837,838)413(841,842)415(845,846)417(849,850)419(853,854)421(857,858)423(861,862)425(865,866)427(869,870)429(873,874)431(877,878)433(881,882)435(885,886)437(889,890)439(893,894)441(897,898)443(901,902)445(905,906)447(909,910)449(913,914)451(917,918)453(921,922)455(925,926)457(929,930)459(933,934)461(937,938)463(941,942)465(945,946)467(949,950)469(953,954)471(957,958)473(961,962)475(965,966)477(969,970)479(973,974)481(977,978)483(981,982)485(985,986)487(989,990)489(993,994)491(997,998)493(1001,1002)495(1005,1006)497(1009,1010)499(1013,1014)501(1017,1018)503(1021,1022)505(1025,1026)507(1029,1030)509(1033,1034)511(1037,1038)513(1041,1042)515(1045,1046)517(1049,1050)519(1053,1054)521(1057,1058)523(1061,1062)525(1065,1066)527(1069,1070)529(1073,1074)531(1077,1078)533(1081,1082)535(1085,1086)537(1089,1090)539(1093,1094)541(1097,1098)543(1101,1102)545(1105,1106)547(1109,1110)549(1113,1114)551(1117,1118)553(1121,1122)555(1125,1126)557(1129,1130)559(1133,1134)561(1137,1138)563(1141,1142)565(1145,1146)567(1149,1150)569(1153,1154)571(1157,1158)573(1161,1162)575(1165,1166)577(1169,1170)579(1173,1174)581(1177,1178)583(1181,1182)585(1185,1186)587(1189,1190)589(1193,1194)591(1197,1198)593(1201,1202)595(1205,1206)597(1209,1210)599(1213,1214)601(1217,1218)603(1221,1222)605(1225,1226)607(1229,1230)609(1233,1234)611(1237,1238)613(1241,1242)615(1245,1246)617(1249,1250)619(1253,1254)621(1257,1258)623(1261,1262)625(1265,1266)627(1269,1270)629(1273,1274)631(1277,1278)633(1281,1282)635(1285,1286)637(1289,1290)639(1293,1294)641(1297,1298)643(1301,1302)645(1305,1306)647(1309,1310)649(1313,1314)651(1317,1318)653(1321,1322)655(1325,1326)657(1329,1330)659(1333,133 |

## Physical Properties

| Property code | Value         | Unit    | Source                                                                                                                                                                         |
|---------------|---------------|---------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| gf            | -8007.70      | kJ/mol  | Joback Method                                                                                                                                                                  |
| hf            | -8867.75      | kJ/mol  | Joback Method                                                                                                                                                                  |
| hfus          | 50.30         | kJ/mol  | Applications of Correlation Gas Chromatography and Transpiration Studies for the Evaluation of the Vaporization and Sublimation Enthalpies of Some Perfluorinated Hydrocarbons |
| hvap          | -0.12         | kJ/mol  | Joback Method                                                                                                                                                                  |
| log10ws       | -15.17        |         | Crippen Method                                                                                                                                                                 |
| logp          | 13.546        |         | Crippen Method                                                                                                                                                                 |
| mcvol         | 367.000       | ml/mol  | McGowan Method                                                                                                                                                                 |
| pc            | 462.88        | kPa     | Joback Method                                                                                                                                                                  |
| tb            | 561.74        | K       | Joback Method                                                                                                                                                                  |
| tc            | 699.59        | K       | Joback Method                                                                                                                                                                  |
| tf            | 437.90 ± 0.50 | K       | NIST Webbook                                                                                                                                                                   |
| tf            | 437.90 ± 0.20 | K       | NIST Webbook                                                                                                                                                                   |
| tf            | 435.60 ± 0.20 | K       | NIST Webbook                                                                                                                                                                   |
| tf            | 443.20 ± 0.20 | K       | NIST Webbook                                                                                                                                                                   |
| vc            | 1.692         | m3/kmol | Joback Method                                                                                                                                                                  |

# Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1277.60 | J/mol×K | 653.64          | Joback Method |
| cpg           | 1300.76 | J/mol×K | 699.59          | Joback Method |
| cpg           | 1289.88 | J/mol×K | 676.62          | Joback Method |
| cpg           | 1211.64 | J/mol×K | 561.74          | Joback Method |
| cpg           | 1230.93 | J/mol×K | 584.72          | Joback Method |
| cpg           | 1248.26 | J/mol×K | 607.69          | Joback Method |
| cpg           | 1263.77 | J/mol×K | 630.67          | Joback Method |
| hfust         | 80.33   | kJ/mol  | 437.90          | NIST Webbook  |
| hfust         | 0.67    | kJ/mol  | 149.50          | NIST Webbook  |
| hfust         | 11.25   | kJ/mol  | 202.90          | NIST Webbook  |
| hfust         | 80.33   | kJ/mol  | 437.90          | NIST Webbook  |
| sfust         | 183.44  | J/mol×K | 437.90          | NIST Webbook  |
| sfust         | 55.45   | J/mol×K | 202.90          | NIST Webbook  |
| sfust         | 4.48    | J/mol×K | 149.50          | NIST Webbook  |

## Sources

Crippen Method:

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

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

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

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

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

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

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C37589574&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  
**hfust:** Enthalpy of fusion at a given temperature  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** Log10 of Water solubility in mol/l

|               |                                          |
|---------------|------------------------------------------|
| <b>logp:</b>  | Octanol/Water partition coefficient      |
| <b>mcvol:</b> | McGowan's characteristic volume          |
| <b>pc:</b>    | Critical Pressure                        |
| <b>sfust:</b> | Entropy of fusion at a given temperature |
| <b>tb:</b>    | Normal Boiling Point Temperature         |
| <b>tc:</b>    | Critical Temperature                     |
| <b>tf:</b>    | Normal melting (fusion) point            |
| <b>vc:</b>    | Critical Volume                          |

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