

**(.+/-.)-Epinephrine,
N,O,O',O''-tetrakis(pentafluoropropionyl)-**

Inchi: InChI=1S/C21H9F20NO7/c1-42(10(43)14(22,23)18(30,31)32)5-9(49-13(46)17(28,29)21(44,45)16(33,34)35(40,41)36(47,48)37(24,25)38(26,27)39(20,21)40(11,12)41(15,16)42(19,20)43(1,2)44(3,4)45(5,6)46(7,8)47(9,10)48(11,12)49(13,14)50(15,16)51(17,18)52(19,20)53(21,22)54(23,24)55(25,26)56(27,28)57(29,30)58(31,32)59(33,34)60(35,36)61(37,38)62(39,40)63(41,42)64(43,44)65(45,46)66(47,48)67(49,50)68(51,52)69(53,54)70(55,56)71(57,58)72(59,60)73(61,62)74(63,64)75(65,66)76(67,68)77(69,70)78(71,72)79(73,74)80(75,76)81(77,78)82(79,80)83(81,82)84(83,84)85(85,86)86(87,88)87(89,90)88(91,92)89(93,94)90(95,96)91(97,98)92(99,100)93(101,102)94(103,104)95(105,106)96(107,108)97(109,110)98(111,112)99(113,114)100(115,116)101(117,118)102(119,120)103(121,122)104(123,124)105(125,126)106(127,128)107(129,130)108(131,132)109(133,134)110(135,136)111(137,138)112(139,140)113(141,142)114(143,144)115(145,146)116(147,148)117(149,150)118(151,152)119(153,154)120(155,156)121(157,158)122(159,160)123(161,162)124(163,164)125(165,166)126(167,168)127(169,170)128(171,172)129(173,174)130(175,176)131(177,178)132(179,180)133(181,182)134(183,184)135(185,186)136(187,188)137(189,190)138(191,192)139(193,194)140(195,196)141(197,198)142(199,200)143(201,202)144(203,204)145(205,206)146(207,208)147(209,210)148(211,212)149(213,214)150(215,216)151(217,218)152(219,220)153(221,222)154(223,224)155(225,226)156(227,228)157(229,230)158(231,232)159(233,234)160(235,236)161(237,238)162(239,240)163(241,242)164(243,244)165(245,246)166(247,248)167(249,250)168(251,252)169(253,254)170(255,256)171(257,258)172(259,260)173(261,262)174(263,264)175(265,266)176(267,268)177(269,270)178(271,272)179(273,274)180(275,276)181(277,278)182(279,280)183(281,282)184(283,284)185(285,286)186(287,288)187(289,290)188(291,292)189(293,294)190(295,296)191(297,298)192(299,300)193(301,302)194(303,304)195(305,306)196(307,308)197(309,310)198(311,312)199(313,314)200(315,316)201(317,318)202(319,320)203(321,322)204(323,324)205(325,326)206(327,328)207(329,330)208(331,332)209(333,334)210(335,336)211(337,338)212(339,340)213(341,342)214(343,344)215(345,346)216(347,348)217(349,350)218(351,352)219(353,354)220(355,356)221(357,358)222(359,360)223(361,362)224(363,364)225(365,366)226(367,368)227(369,370)228(371,372)229(373,374)230(375,376)231(377,378)232(379,380)233(381,382)234(383,384)235(385,386)236(387,388)237(389,390)238(391,392)239(393,394)240(395,396)241(397,398)242(399,400)243(401,402)244(403,404)245(405,406)246(407,408)247(409,410)248(411,412)249(413,414)250(415,416)251(417,418)252(419,420)253(421,422)254(423,424)255(425,426)256(427,428)257(429,430)258(431,432)259(433,434)260(435,436)261(437,438)262(439,440)263(441,442)264(443,444)265(445,446)266(447,448)267(449,450)268(451,452)269(453,454)270(455,456)271(457,458)272(459,460)273(461,462)274(463,464)275(465,466)276(467,468)277(469,470)278(471,472)279(473,474)280(475,476)281(477,478)282(479,480)283(481,482)284(483,484)285(485,486)286(487,488)287(489,490)288(491,492)289(493,494)290(495,496)291(497,498)292(499,500)293(501,502)294(503,504)295(505,506)296(507,508)297(509,510)298(511,512)299(513,514)300(515,516)301(517,518)302(519,520)303(521,522)304(523,524)305(525,526)306(527,528)307(529,530)308(531,532)309(533,534)310(535,536)311(537,538)312(539,540)313(541,542)314(543,544)315(545,546)316(547,548)317(549,550)318(551,552)319(553,554)320(555,556)321(557,558)322(559,560)323(561,562)324(563,564)325(565,566)326(567,568)327(569,570)328(571,572)329(573,574)330(575,576)331(577,578)332(579,580)333(581,582)334(583,584)335(585,586)336(587,588)337(589,590)338(591,592)339(593,594)340(595,596)341(597,598)342(599,600)343(601,602)344(603,604)345(605,606)346(607,608)347(609,610)348(611,612)349(613,614)350(615,616)351(617,618)352(619,620)353(621,622)354(623,624)355(625,626)356(627,628)357(629,630)358(631,632)359(633,634)360(635,636)361(637,638)362(639,640)363(641,642)364(643,644)365(645,646)366(647,648)367(649,650)368(651,652)369(653,654)370(655,656)371(657,658)372(659,660)373(661,662)374(663,664)375(665,666)376(667,668)377(669,670)378(671,672)379(673,674)380(675,676)381(677,678)382(679,680)383(681,682)

Physical Properties

Property code	Value	Unit	Source
gf	-4376.73	kJ/mol	Joback Method
hf	-5040.11	kJ/mol	Joback Method
hfus	55.15	kJ/mol	Joback Method
hvap	75.10	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	6.330		Crippen Method
mcvol	352.260	ml/mol	McGowan Method
pc	828.59	kPa	Joback Method
rinpol	1540.00		NIST Webbook
tb	970.82	K	Joback Method
tc	1213.39	K	Joback Method
tf	692.93	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1174.43	J/mol×K	970.82	Joback Method
cpg	1184.03	J/mol×K	1011.25	Joback Method
cpg	1193.01	J/mol×K	1051.68	Joback Method
cpg	1201.68	J/mol×K	1092.11	Joback Method
cpg	1210.31	J/mol×K	1132.53	Joback Method
cpg	1219.22	J/mol×K	1172.96	Joback Method
cpg	1228.68	J/mol×K	1213.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375691&Units=SI
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

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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