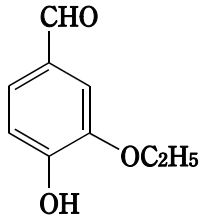
Chemical Name;3-Ethoxy-4-hydroxybenzaldehyde
Synonym ;Ethyl vanillin
Vanillal
4-Hydoxy-3-ethoxybenzaldehyde
ｴﾁﾙﾊﾞﾆﾘﾝ
ﾊﾞﾆﾗｰﾙ
4-ﾋﾄﾞﾛｷｼ-3-ｴﾄｷｼﾍﾞﾝｽﾞｱﾙﾃﾞﾋﾄﾞ

Molecular Weight ; 166.18
Melting Point ; 76 - 78 ℃ [CHCD,Aldrich]
77 - 78 ℃ [Merck]
Boiling Point ; — ℃
Flashing Point ; — ℃
Molecular Formula; $C_9H_{10}O_3$

Chemical Structure



CAS No. ; 121-32-4
MITI No. ; (3)-1201
ML No. ; —
Specified Chemical Substances; —

Source of Substance; Tokyo Kasei Kogyo Co.,Ltd.
Lot No. ; AX01
Purity ; 98 %

Vehicle ; DMSO

Mutagenicity in Bacterial Test ; **Negative**

IARC Evaluation ; not yet cited

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvrA*		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(120)	(138)	(14)	(17)	(34)	(27)	(12)	(21)	(6)	(8)
	149	136	11	18	20	36	11	18	5	7
	119	163	21	20	33	37	11	23	3	11
0.0763	(134)	(150)	(16)	(19)	(27)	(37)	(11)	(21)	(4)	(9)
	123	134	18	11	30	33	10	14	6	7
	128	146	22	16	43	39	14	17	6	8
0.305	(126)	(140)	(20)	(14)	(37)	(36)	(12)	(16)	(6)	(8)
	143	141	13	20	33	26	23	22	5	6
	122	155	14	11	24	37	9	21	6	7
1.22	(133)	(148)	(14)	(16)	(29)	(32)	(16)	(22)	(6)	(7)
	112	124	13	23	39	39	14	15	5	6
	138	136	15	15	26	29	13	15	3	6
4.88	(125)	(130)	(14)	(19)	(33)	(34)	(14)	(15)	(4)	(6)
	112	159	14	15	30	26	14	24	6	10
	134	156	20	10	32	43	17	16	8	9
19.5	(123)	(158)	(17)	(13)	(31)	(35)	(16)	(20)	(7)	(10)
	106	138	10	17	43	36	11	26	7	7
	113	143	10	18	36	41	10	25	7	7
78.1	(110)	(141)	(10)	(18)	(40)	(39)	(11)	(26)	(7)	(7)
	98	146	20	11	31	33	15	28	6	11
	112	179	13	16	34	37	13	28	5	8
313	(105)	(163)	(17)	(14)	(33)	(35)	(14)	(28)	(6)	(10)
	121	136	15	7	33	33	9	28	5	13
	86	131	15	18	26	32	13	20	3	11
1250	(104)	(134)	(15)	(13)	(30)	(33)	(11)	(24)	(4)	(12)
	75	90*	13	14*	26	36	9	18	5	5*
	83	90*	8	9*	30	31	10	20	5	10*
5000	(79)	(90*)	(11)	(12*)	(28)	(34)	(10)	(19)	(5)	(8*)
Judgement	—	—	—	—	—	—	—	—	—	—
Specific Mutagenicity										
Positive Control	AF-2 (845)	2-AA (1045)	NaN_3 (392)	2-AA (337)	AF-2 (277)	2-AA (1158)	AF-2 (313)	2-AA (246)	9-AA (680)	2-AA (168)

Conc. μg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvrA*		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(132)	(133)	(18)	(17)	(26)	(32)	(15)	(23)	(13)	(15)
	106	152	17	20	28	43	8	24	10	10
	102	144	15	24	14	44	10	16	7	16
78.1	(104)	(148)	(16)	(22)	(21)	(44)	(9)	(20)	(9)	(13)
	109	157	11	22	26	39	22	23	9	17
	136	144	8	18	38	39	15	17	8	8
156	(123)	(151)	(10)	(20)	(32)	(39)	(19)	(20)	(9)	(13)
	105	173	7	15	31	32	8	18	13	10
	115	150	16	21	28	38	10	32	14	18
313	(110)	(162)	(12)	(18)	(30)	(35)	(9)	(25)	(14)	(14)
	113	155	18	18	33	52	10	29	14	21
	111	144	20	21	32	54	7	32	13	21
625	(112)	(150)	(19)	(20)	(33)	(53)	(9)	(31)	(14)	(21)
	119	165	13	9	30	45	16	23	16	21
	98	169	8	11	31	44	8	18	7	10
1250	(109)	(167)	(11)	(10)	(31)	(45)	(12)	(21)	(12)	(16)
	97	123	9	15	26	47	15	26	5	8
	119	141	18	8	26	41	7	20	14	15
2500	(108)	(132)	(14)	(12)	(26)	(44)	(11)	(23)	(10)	(12)
	84	99*	7	9*	17	33	9	17	5	9*
	63	87*	8	8*	20	34	8	13	16	16*
5000	(74)	(93*)	(8)	(9*)	(19)	(34)	(9)	(15)	(11)	(13*)
Judgement	−	−	−	−	−	−	−	−	−	−
Specific Mutagenicity										
Positive Control	AF-2 (809)	2-AA (1456)	NaN_3 (375)	2-AA (285)	AF-2 (354)	2-AA (1520)	AF-2 (475)	2-AA (376)	9-AA (739)	2-AA (275)

Experimental Data - 3

Conc. μg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2*uvrA*/pKM101	
	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(204)	(276)	(262)	(313)	(32)	(53)
	207	288	236	313	26	46
	201	239	238	355	24	64
0.0763	(204)	(264)	(237)	(334)	(25)	(55)
	200	290	250	335	29	56
	222	293	241	349	39	70
0.305	(211)	(292)	(246)	(342)	(34)	(63)
	204	287	255	320	26	46
	205	252	241	340	24	68
1.22	(205)	(270)	(248)	(330)	(25)	(57)
	197	303	250	364	31	57
	239	287	238	335	23	66
4.88	(218)	(295)	(244)	(350)	(27)	(62)
	209	330	260	405	29	62
	195	295	232	366	36	56
19.5	(202)	(313)	(246)	(386)	(33)	(59)
	188	293	271	335	34	66
	205	304	261	337	28	61
78.1	(197)	(299)	(266)	(336)	(31)	(64)
	194	318	242	335	43	66
	183	317	242	320	33	54
313	(189)	(318)	(242)	(328)	(38)	(60)
	141	303	187	290	25	67
	142	284	221	249	32	53
1250	(142)	(294)	(204)	(270)	(29)	(60)
	30*	38*	185	245*	16	25
	21*	54*	183	221*	18	23
5000	(26*)	(46*)	(184)	(233*)	(17)	(24)
Judgement	−	−	−	−	−	−
Specific Mutagenicity						
Positive Control	BLM (807)	2-AA (2129)	PA (1644)	2-AA (1204)	AF-2 (1466)	2-AA (1022)

Experimental Data - 4

Conc. μg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2*uvrA*/pKM101	
	S9−	S9+	S9−	S9+	S9−	S9+
DMSO	(245)	(282)	(213)	(305)	(50)	(76)
	252	314	201	332	30	70
	233	299	223	318	46	74
78.1	(243)	(307)	(212)	(325)	(38)	(72)
	236	317	226	297	40	61
	216	332	199	336	51	82
156	(226)	(325)	(213)	(317)	(46)	(72)
	211	292	174	319	48	91
	212	310	219	341	45	87
313	(212)	(301)	(197)	(330)	(47)	(89)
	258	300	216	350	51	67
	221	316	180	325	51	62
625	(240)	(308)	(198)	(338)	(51)	(65)
	199	260	149	341	46	72
	183	294	151	307	37	72
1250	(191)	(277)	(150)	(324)	(42)	(72)
	186	223	104	256	51	67
	164	211	98	248	40	70
2500	(175)	(217)	(101)	(252)	(46)	(69)
	198	34*	31	162*	31	41
	216	37*	28	214*	30	44
5000	(207)	(36*)	(30)	(188*)	(31)	(43)
Judgement	−	−	−	−	−	−
Specific Mutagenicity						
Positive Control	BLM (773)	2-AA (1626)	PA (1601)	2-AA (1203)	AF-2 (1060)	2-AA (942)