Chemical Name; Butyl acetate
Synonym ; *n*-Butyl acetate
Acetic acid *n*-butyl ester

Molecular Weight ; 116.16
Melting Point ; - 78 ℃ [Aldrich]
- 77 ℃ [Merck]
Boiling Point ; 125 - 126 ℃ [CHCD;Merck]
124 - 126 ℃ [Aldrich]
Flashing Point ; 22 ℃ [CHCD;Aldrich;
Merck(c.c.)]
Molecular Formula; $C_6H_{12}O_2$

Chemical Structure

$CH_3COOCH_2CH_2CH_2CH_3$

CAS No. ; 123-86-4
MITI No. ; (2)-731
ML No. ; 2-(6)-226
Specified Chemical Substances; —

Source of Substance; Tokyo Kasei Kogyo Co.,Ltd.
Lot No. ; FHC01
Purity ; ≧ 99 %

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	(119)	(138)	(9)	(8)	(25)	(31)	(15)	(26)	(7)	(12)
	100	142	6	6	32	33	14	26	6	7
	141	126	16	8	28	37	24	28	6	18
0.0763	(121)	(134)	(11)	(7)	(30)	(35)	(19)	(27)	(6)	(13)
	134	149	9	7	33	31	15	32	5	7
	142	123	13	10	23	34	13	25	7	14
0.305	(138)	(136)	(11)	(9)	(28)	(33)	(14)	(29)	(6)	(11)
	99	138	14	8	29	26	8	17	6	17
	133	159	9	8	21	30	17	18	6	8
1.22	(116)	(149)	(12)	(8)	(25)	(28)	(13)	(18)	(6)	(13)
	116	142	7	8	30	33	24	18	3	10
	111	116	9	11	39	33	9	21	7	8
4.88	(114)	(129)	(8)	(10)	(35)	(33)	(17)	(20)	(5)	(9)
	104	117	9	14	25	26	15	28	7	9
	129	115	9	11	25	33	20	22	11	3
19.5	(117)	(116)	(9)	(13)	(25)	(30)	(18)	(25)	(9)	(6)
	117	134	8	10	15	32	20	34	11	10
	123	126	10	7	32	29	29	21	6	6
78.1	(120)	(130)	(9)	(9)	(24)	(31)	(25)	(28)	(9)	(8)
	117	115	10	10	25	30	16	24	6	9
	126	128	14	9	30	32	10	17	2	11
313	(122)	(122)	(12)	(10)	(28)	(31)	(13)	(21)	(4)	(10)
	141	143	8	9	23	36	25	21	6	15
	108	129	9	10	8	32	10	20	9	13
1250	(125)	(136)	(9)	(10)	(16)	(34)	(18)	(21)	(8)	(14)
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
5000	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
Judgement	—	—	—	—	—	—	—	—	—	—
Specific Mutagenicity										
Positive Control	AF-2 (871)	2-AA (1263)	NaN_3 (348)	2-AA (322)	AF-2 (390)	2-AA (1114)	AF-2 (563)	2-AA (332)	9-AA (721)	2-AA (240)

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	(110)	(116)	(9)	(8)	(21)	(26)	(17)	(26)	(6)	(10)
2.44			5 6 (6)	10 8 (9)			18 15 (17)	23 40 (32)		
4.88			10 5 (8)	8 17 (13)			14 24 (19)	28 21 (25)		
9.77			10 7 (9)	15 7 (11)			10 15 (13)	22 33 (28)		
19.5			7 9 (8)	11 8 (10)			14 16 (15)	30 25 (28)		
39.1			9 15 (12)	8 9 (9)			15 24 (20)	34 34 (34)		
78.1	92 120 (106)	128 129 (129)	6 8 (7)	7 11 (9)	24 15 (20)	23 28 (26)	17 20 (19)	20 30 (25)	6 3 (5)	9 6 (8)
156	104 127 (116)	116 109 (113)	7 6 (7)	10 5 (8)	21 16 (19)	43 32 (38)	21 16 (19)	31 23 (27)	5 5 (5)	6 14 (10)
313	89 100 (95)	129 129 (129)	8 9 (9)	10 10 (10)	22 25 (24)	36 22 (29)	10 13 (12)	31 24 (28)	7 5 (6)	7 8 (8)
625	116 106 (111)	131 123 (127)	8 3 (6)	13 10 (12)	10 24 (17)	25 26 (26)	11 15 (13)	23 17 (20)	3 5 (4)	13 7 (10)
1250	107 108 (108)	122 134 (128)	9 5 (7)	9 6 (8)	29 17 (23)	29 24 (27)	13 9 (11)	24 26 (25)	3 5 (4)	7 10 (9)
2500	85* 77* (81*)	135 126 (131)	5* 2* (4*)	7 7 (7)	21 23 (22)	24 26 (25)	11* 15* (13*)	15 29 (22)	1* 5* (3*)	10 7 (9)
5000	0* 0* (0*)	0* 0* (0*)	0* 0* (0*)	0* 0* (0*)	0* 0* (0*)	0* 0* (0*)	0* 0* (0*)	0* 0* (0*)	0* 0* (0*)	0* 0* (0*)
Judgement	−	−	−	−	−	−	−	−	−	−
Specific Mutagenicity										
Positive Control	AF-2 (723)	2-AA (1033)	NaN_3 (318)	2-AA (295)	AF-2 (263)	2-AA (1077)	AF-2 (509)	2-AA (259)	9-AA (789)	2-AA (169)

Experimental Data - 3

Conc. μg/plate	Number of Revertants/plate Base-substitution TA102 S9−	TA102 S9+	TA104 S9−	TA104 S9+	WP2*uvrA*/pKM101 S9−	WP2*uvrA*/pKM101 S9+
DMSO	(237)	(302)	(313)	(320)	(47)	(82)
	235	288	311	360	39	66
	234	314	319	373	38	70
0.0763	(235)	(301)	(315)	(367)	(39)	(68)
	243	281	290	365	39	70
	235	287	303	335	48	77
0.305	(239)	(284)	(297)	(350)	(44)	(74)
	238	325	282	349	37	76
	230	261	336	350	49	78
1.22	(234)	(293)	(309)	(350)	(43)	(77)
	222	287	338	361	54	81
	261	293	323	366	61	69
4.88	(242)	(290)	(331)	(364)	(58)	(75)
	261	305	298	353	45	66
	249	330	276	370	47	72
19.5	(255)	(318)	(287)	(362)	(46)	(69)
	239	341	279	352	32	79
	228	280	260	340	45	77
78.1	(234)	(311)	(270)	(346)	(39)	(78)
	259	299	287	348	46	72
	222	249	294	328	46	74
313	(241)	(274)	(291)	(338)	(46)	(73)
	234	301	305	320	46	59
	252	292	324	341	51	66
1250	(243)	(297)	(315)	(331)	(49)	(63)
	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*
5000	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
Judgement	−	−	−	−	−	−
Specific Mutagenicity						
Positive Control	BLM (763)	2-AA (992)	PA (1407)	2-AA (1105)	AF-2 (1227)	2-AA (915)

Experimental Data - 4

Conc. μg/plate	Number of Revertants/plate Base-substitution TA102 S9−	TA102 S9+	TA104 S9−	TA104 S9+	WP2*uvrA*/pKM101 S9−	WP2*uvrA*/pKM101 S9+
DMSO	(239)	(297)	(311)	(379)	(44)	(61)
	249	299	324	399	45	60
	269	274	265	436	43	75
78.1	(259)	(287)	(295)	(418)	(44)	(68)
	242	296	336	411	52	61
	242	305	318	391	37	56
156	(242)	(302)	(327)	(401)	(45)	(59)
	249	314	294	413	43	74
	282	331	280	397	43	97
313	(266)	(323)	(287)	(405)	(43)	(86)
	239	300	335	459	43	75
	258	311	354	335	48	77
625	(249)	(306)	(345)	(397)	(46)	(76)
	242	294	328	378	55	57
	226	281	364	388	51	64
1250	(234)	(288)	(346)	(383)	(53)	(61)
	212	249*	278*	352*	26*	70*
	180	246*	312*	354*	32*	72*
2500	(196)	(248*)	(295*)	(353*)	(29*)	(71*)
	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*
5000	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
Judgement	−	−	−	−	−	−
Specific Mutagenicity						
Positive Control	BLM (789)	2-AA (2211)	PA (2477)	2-AA (1115)	AF-2 (1231)	2-AA (1086)