

Benzyl mercaptan

[ベンジールメルカプタン]

Experimental Data - 1

(B9318-1/3)

Chemical Name; Benzyl mercaptan
 Synonym ; 2-Mercaptotoluene
 Thiobenzyl alcohol
 Benzenemethanethiol
 Benzyl thiol
 (Thiomethyl)benzene
 2-メルカプトトルエン
 チオベンジールアルコール
 ベンゼンメタンチオール
 ベンジールチオール
 チオメチルベンゼン

Molecular Weight ; 124.21

Melting Point ; - ℃

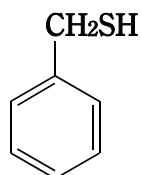
Boiling Point ; 194 - 195 ℃

[CHCD, Aldrich, Merck]

Flashing Point ; 70 ℃ [Aldrich]

Molecular Formula; C₇H₈S

Chemical Structure



CAS No. ; 100-53-8

MITI No. ; (3)-1105

ML No. ; 4-(10)-576

Specified Chemical Substances; -

Source of Substance; Tokyo Kasei Kogyo Co., Ltd.

Lot No. ; FIB01

Purity ; 99.1 %

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		WP2uvrA		TA98		TA1537	
	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
DMSO	(133)	(139)	(15)	(12)	(26)	(29)	(18)	(26)	(7)	(11)
	157	148	16	16	26	29	13	24	7	17
	131	167	11	15	20	31	9	32	9	9
0.0763	(144)	(158)	(14)	(16)	(23)	(30)	(11)	(28)	(8)	(13)
	178	126	18	17	20	24	18	22	7	14
	164	120	18	9	18	25	6	25	8	9
0.305	(171)	(123)	(18)	(13)	(19)	(25)	(12)	(24)	(8)	(12)
	129	107	8	13	25	29	15	11	7	9
	124	131	15	10	24	30	18	24	9	8
1.22	(127)	(119)	(12)	(12)	(25)	(30)	(17)	(18)	(8)	(9)
	173	142	16	6	26	47	10	22	10	11
	172	130	15	14	26	39	18	21	9	11
4.88	(173)	(136)	(16)	(10)	(26)	(43)	(14)	(22)	(10)	(11)
	141	139	14	14	21	31	22	30	13	6
	178	121	8	14	28	34	13	29	3	14
19.5	(160)	(130)	(11)	(14)	(25)	(33)	(18)	(30)	(8)	(10)
	143	141*	5*	7*	26	31	16	33	5	11*
	148	127*	14*	9*	28	33	15	29	6	14*
78.1	(146)	(134*)	(10*)	(8*)	(27)	(32)	(16)	(31)	(6)	(13*)
	0*	96*	0*	0*	0*	31*	7*	13*	0*	0*
	0*	79*	0*	0*	0*	23*	6*	15*	0*	0*
313	(0*)	(88*)	(0*)	(0*)	(0*)	(27*)	(7*)	(14*)	(0*)	(0*)
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
1250	(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*
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 (741)	2-AA (980)	NaN ₃ (375)	2-AA (263)	AF-2 (144)	2-AA (1216)	AF-2 (582)	2-AA (291)	9-AA (477)	2-AA (130)

Conc. µg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA		TA98		TA1537	
	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
	(138)	(119)	(13)	(15)	(29)	(35)	(16)	(27)	(8)	(11)
DMSO	145	135	8	17						9
	135	149	14	13						9
1. 22	(140)	(142)	(11)	(15)						(9)
	129	116	13	16	20				7	13
	150	137	11	10	23				6	7
2. 44	(140)	(127)	(12)	(13)	(22)				(7)	(10)
	124	135	18	10	24	32	15	28	9	8
	124	124	18	8	36	33	17	28	6	9
4. 88	(124)	(130)	(18)	(9)	(30)	(33)	(16)	(28)	(8)	(9)
	128	150	9	14	32	30	11	24	10	17
	119	122	10	11	28	36	13	15	8	6
9. 77	(124)	(136)	(10)	(13)	(30)	(33)	(12)	(20)	(9)	(12)
	137	135	15	14	22	39	13	17	9	10
	130	100	9	13	31	31	14	33	6	7
19. 5	(134)	(118)	(12)	(14)	(27)	(35)	(14)	(25)	(8)	(9)
	116	133	6	7	22	38	20	23	11	10
	102	144	5	11	30	31	16	28	11	5
39. 1	(109)	(139)	(6)	(9)	(26)	(35)	(18)	(26)	(11)	(8)
	101	98*	15*	14*	28	32	16	26	6	8*
	101	136*	10*	15*	29	25	10	20	6	11*
78. 1	(101)	(117*)	(13*)	(15*)	(29)	(29)	(13)	(23)	(6)	(10*)
	77*	112*	6*	7*	15	37	17	23	6*	8*
	85*	85*	11*	6*	21	26	11	14	3*	5*
156	(81*)	(99*)	(9*)	(7*)	(18)	(32)	(14)	(19)	(5*)	(7*)
					0*	30*	8*	15*	0*	
					0*	22*	7*	11*	0*	
313					(0*)	(26*)	(8*)	(13*)	(0*)	
						14*	0*	0*		
						10*	0*	0*		
625						(12*)	(0*)	(0*)		
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 (822)	2-AA (984)	NaN ₃ (394)	2-AA (270)	AF-2 (178)	2-AA (1290)	AF-2 (544)	2-AA (304)	9-AA (700)	2-AA (172)

Experimental Data - 3

Conc. µg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2uvrA/pKM101	
	S9-	S9+	S9-	S9+	S9-	S9+
DMSO	(316)	(393)	(298)	(359)	(60)	(85)
	334	425	297	352	68	92
	325	382	275	373	56	89
0.0763	(330)	(404)	(286)	(363)	(62)	(91)
	340	408	286	353	52	81
	324	373	307	360	47	76
0.305	(332)	(391)	(297)	(357)	(50)	(79)
	337	397	313	319	60	70
	312	483	295	332	56	69
1.22	(325)	(440)	(304)	(326)	(58)	(70)
	300	355	330	342	63	89
	318	387	255	318	74	85
4.88	(309)	(371)	(293)	(330)	(69)	(87)
	313	382	255	303	51	79
	319	378	312	314	54	90
19.5	(316)	(380)	(284)	(309)	(53)	(85)
	252	256	276	255	63	56
	292	263	260	221	63	82
78.1	(272)	(260)	(268)	(238)	(63)	(69)
	153*	260	0*	236*	0*	63
	126*	235	0*	238*	0*	63
313	(140*)	(248)	(0*)	(237*)	(0*)	(63)
	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*
1250	(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*)

Judgement — — — — —

Specific Mutagenicity

Positive Control	BLM	2-AA	PA	2-AA	AF-2	2-AA
	(907)	(1399)	(1805)	(1238)	(784)	(1077)

Experimental Data - 4

(B9318-3/3)

Conc. µg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2uvrA/pKM101	
	S9-	S9+	S9-	S9+	S9-	S9+
DMSO	(289)	(357)	(290)	(362)	(60)	(86)
	306		274		36	
	295		306		51	
4.88	(301)		(290)		(44)	
	324		304	382	68	
	293		295	347	48	
9.77	(309)		(300)	(365)	(58)	
	297	349	281	335	67	63
	281	329	260	373	57	85
19.5	(289)	(339)	(271)	(354)	(62)	(74)
	282	286	254	366	57	75
	274	293	249	358	53	82
39.1	(278)	(290)	(252)	(362)	(55)	(79)
	284	238	288	220	54	55
	254	239	276	234	53	74
78.1	(269)	(239)	(282)	(227)	(54)	(65)
	263	238	295	230	51	84
	281	200	250	177	44	85
156	(272)	(219)	(273)	(204)	(48)	(85)
	121*	215	0*	239*	0*	81
	107*	233	0*	230*	0*	72
313	(114*)	(224)	(0*)	(235*)	(0*)	(77)
		0*		0*		0*
		0*		0*		0*
625		(0*)		(0*)		(0*)
		0*				0*
		0*				0*
1250		(0*)				(0*)

Judgement — — — — —

Specific Mutagenicity

Positive Control	BLM	2-AA	PA	2-AA	AF-2	2-AA
	(950)	(1306)	(2002)	(1105)	(1453)	(894)