

n-Octylbromide (n-オクチルブロミド)

Chemical Name: n-Octylbromide
 Synonym: 1-Bromooctane
 Octane, 1-bromo-
 Molecular weight: 193.13
 Melting point: -55°C
 Boiling point: 201.5°C
 Flashing point: 78°C
 Chemical Structure

$$\text{CH}_3 (\text{CH}_2)_7 \text{Br}$$

 CAS NO : 111-83-1
 MITI NO: (2)-67
 Source of Substance: Tokyo Kasei Kogyo Co. Ltd
 Lot. No. : FAX01
 Purity: ≥ 98 %
 Vehicle: DMSO

Mutagenicity
 in Bacterial Test : Negative

IARC Evaluation : not yet cited

Con. μg/ plate	Experimental Data									
	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA		TA98		TA1537	
	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
DMSO	(184)	(177)	(9)	(11)	(28)	(36)	(18)	(25)	(6)	(12)
	198		8				20		11	
	149		8				17		6	
0.0610	(174)		(8)				(19)		(9)	
	173		8		23		20		11	
	188		10		31		11		10	
0.122	(181)		(9)		(27)		(16)		(11)	
	170		6		37		15		8	
	155		11		32		22		6	
0.244	(163)		(9)		(35)		(19)		(7)	
	169	143	9	11	30		16		7	
	151	181	11	6	32		13		8	
0.488	(160)	(162)	(10)	(9)	(31)		(15)		(8)	
	153	159	10	9	34		14	21	8	9
	160	149	13	11	29		20	21	6	10
0.977	(157)	(154)	(12)	(10)	(32)		(17)	(21)	(7)	(10)
	119	177	8	7	21	34	22	18	7	14
	109	192	10	15	25	34	13	26	11	13
1.95	(114)	(185)	(9)	(11)	(23)	(34)	(18)	(22)	(9)	(14)
	67*	171	2*	10	25	39	13	13	3*	10
	87*	192	5*	16	32	32	10	31	5*	5
3.91	(77*)	(182)	(4*)	(13)	(29)	(36)	(12)	(22)	(4*)	(8)
	68*	146	6*	8	28*	32	10*	26	3*	15
	51*	163	6*	13	21*	38	15*	26	3*	11
7.81	(60*)	(155)	(6*)	(11)	(25*)	(35)	(13*)	(26)	(3*)	(13)
	48*	177	6*	15	31*	37	10*	26	0*	13
	52*	151	6*	13	23*	39	10*	28	0*	13
15.6	(50*)	(164)	(6*)	(14)	(27*)	(38)	(10*)	(27)	(0*)	(13)
		150		16	21*	34		24		10
		143		7	23*	37		20		15
31.3		(162)		(12)	(22*)	(36)		(22)		(13)

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Experimental Data										
Con. μ g/ plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA		TA98		TA1537	
	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
		74*		11*		37		22		15
		74*		15*		41		21		9
<u>62.5</u>		(74*)		(13*)		(39)		(22)		(12)
		63*		0*		22		13*		8*
		59*		0*		40		14*		10*
<u>125</u>		(61*)		(13*)		(31)		(14*)		(9*)
						40*		0*		13*
						23*		0*		10*
<u>250</u>						(32*)		(0)		(12*)
						37*				
						31*				
<u>500</u>						(34*)				
Judgement	—	—	—	—	—	—	—	—	—	—
Specific Mutagenicity										
Positive	AF2	2AA	NaN ₃	2AA	AF2	2AA 20	AF2	2AA	9AA	2AA
Control	(593)	(832)	(298)	(167)	(169)	(1500)	(418)	(413)	(271)	(128)

Experimental Data										
Con. μ g/ plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2uvrA		TA98		TA1537	
	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+	S9-	S9+
<u>DMSO</u>	(159)	(146)	(9)	(9)	(28)	(37)	(38)	(33)	(7)	(15)
	184		10						7	
	169		10						6	
<u>0.0610</u>	(177)		(10)						(7)	
	193		11		28		54		3	
	190		9		25		32		5	
<u>0.122</u>	(192)		(10)		(27)		(43)		(4)	
	150		8		39		25		7	
	152		8		28		28		9	
<u>0.244</u>	(151)		(8)		(34)		(27)		(8)	
	152		9		33		30		7	
	172		3		34		30		8	
<u>0.488</u>	(162)		(6)		(34)		(30)		(8)	
	155	139	13	13	28		43		8	
	174	185	9	13	23		32		7	
<u>0.977</u>	(165)	(162)	(11)	(13)	(26)		(38)		(8)	
	170	148	9	10	29		25	36	8	16
	139	145	8	5	38		30	32	8	10
<u>1.95</u>	(155)	(147)	(9)	(8)	(34)		(28)	(34)	(8)	(13)
	90*	139	5*	13	32	29	32	34	5*	15
	98*	163	2*	11	26	34	25	32	8*	11
<u>3.91</u>	(94*)	(151)	(4*)	(12)	(29)	(32)	(29)	(33)	(7*)	(13)
		133		9	30*	49	13*	39		7
		167		13	30*	36	21*	37		16
<u>7.81</u>		(150)		(11)	(30*)	(43)	(17*)	(38)		(12)
		144		13		53		36		14
		180		14		45		39		16
<u>15.6</u>		(162)		(14)		(49)		(38)		(15)

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Experimental Data										
Con. 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+
		129		11		41		33		13
		128		14		49		29		13
<u>31.3</u>		(129)		(13)		(45)		(31)		(13)
		104*		10*		44		31		16
		98*		8*		34		26		15
<u>62.5</u>		(101*)		(9*)		(39)		(29)		(16)
						44		31*		13*
						44		39*		11*
<u>125</u>						(44)		(35*)		(12*)
						34*				
						44				
<u>250</u>						(39*)				
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive	AF2	2AA	NaN ₃	2AA	AF2	2AA 20	AF2	2AA	9AA	2AA
Control	(509)	(587)	(232)	(119)	(194)	(1382)	(367)	(374)	(267)	(103)

Experimental Data						
Con. μ g/ plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2uvrA/pKM101	
	S9-	S9+	S9-	S9+	S9-	S9+
<u>Acetone</u>	(250)	(317)	(282)	(403)	(108)	(141)
	273		287		106	
	238		269		99	
<u>0.0305</u>	(256)		(278)		(103)	
	252		303		117	
	263		291		93	
<u>0.0610</u>	(258)		(297)		(105)	
	250		318		112	
	250		290		112	
<u>0.122</u>	(250)		(304)		(112)	
	279	322	300	365	100	
	258	344	323	366	93	
<u>0.244</u>	(269)	(333)	(312)	(366)	(97)	
	279	318	304	419	113	
	243	306	294	338	106	
<u>0.488</u>	(261)	(312)	(299)	(379)	(110)	
	239	313	298	412	113	135
	234	285	303	372	108	149
<u>0.977</u>	(237)	(299)	(301)	(392)	(111)	(142)
	262	343	297	374	107	151
	256	320	290	421	108	159
<u>1.95</u>	(259)	(332)	(294)	(398)	(108)	(155)
	247	326	288	401	117	157
	232	300	290	411	104	152
<u>3.91</u>	(240)	(313)	(289)	(406)	(111)	(155)
	180*	328	218*	414	83*	127
	160*	334	228*	390	89*	130
<u>7.81</u>	(170*)	(331)	(223*)	(402)	(86*)	(129)
	83*	331	166*	425	94*	159
	112*	312	170*	422	75*	145
<u>15.6</u>	(98*)	(322)	(168*)	(424)	(85*)	(152)

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Con. μ g/ plate	Experimental Data					
	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2uvra/pkM101	
	S9-	S9+	S9-	S9+	S9-	S9+
		312		436		128
		316		391		141
<u>31.3</u>		(314)		(414)		(135)
		314		353		143
		311		320		153
<u>62.5</u>		(313)		(337)		(148)
		226*		152*		139
		202*		137*		130
<u>125</u>		(214*)		(145*)		(135)
						123
						156
<u>250</u>						(140)
						119*
						108*
<u>500</u>						(114*)
Judgement	—	—	—	—	—	—
Specific Mutagenicity						
Positive	BLM	2AA	PA	2AA	AF2	2AA
Control	(627)	(1206)	(2019)	(1419)	(680)	(643)