

1-Octanol
[1-オクタノール]

Experimental Data - 1

(B9409-1/3)

Chemical Name; 1-Octanol
 Synonym ; *n*-Capryl alcohol
 n-Octyl alcohol
 n-カプリルアルコール
 n-オクチルアルコール
 Molecular Weight ; 130.23
 Melting Point ; - 16.7 °C [CHCD]
 - 15 °C [Aldrich]
 - 16 - - 17 °C [Merck]
 Boiling Point ; 194.45 °C, 98 °C (19mmHg) [CHCD]
 196 °C [Aldrich]
 194 - 195 °C [Merck]
 Flashing Point ; 81 °C [Aldrich]
 Molecular Formula; C₈H₁₈O
 Chemical Structure

CH₃(CH₂)₆CH₂OH

 CAS No. ; 111-87-5
 MITI No. ; (2)-217
 ML No. ; -
 Specified Chemical Substances; -

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

 Vehicle ; DMSO

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	(156)	(152)	(20)	(15)	(34)	(41)	(18)	(22)	(6)	(9)
	164	135	19	17	26	39	14	23	5	16
	141	137	23	16	37	31	18	34	2	6
0.0763	(153)	(136)	(21)	(17)	(32)	(35)	(16)	(29)	(4)	(11)
	141	135	32	14	29	52	14	24	7	7
	122	137	25	14	37	38	18	24	2	8
0.305	(132)	(136)	(29)	(14)	(33)	(45)	(16)	(24)	(5)	(8)
	141	138	31	29	28	43	20	28	5	13
	109	139	25	15	31	36	13	20	8	7
1.22	(125)	(139)	(28)	(22)	(30)	(40)	(17)	(24)	(7)	(10)
	162	124	11	11	38	39	14	22	3	8
	134	109	27	13	39	36	17	29	6	7
4.88	(148)	(117)	(19)	(12)	(39)	(38)	(16)	(26)	(5)	(8)
	148	111	20	20	30	34	20	16	6	8
	139	121	29	20	41	45	25	30	3	8
19.5	(144)	(116)	(25)	(20)	(36)	(40)	(23)	(23)	(5)	(8)
	135*	123*	29*	15	31*	45	23	24	5	6
	116*	119*	32*	17	24*	36	15	26	5	6
78.1	(126*)	(121*)	(31*)	(16)	(28*)	(41)	(19)	(25)	(5)	(6)
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*	0*	0*	0*	0*
313	(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*
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 (892)	2-AA (1517)	NaN ₃ (434)	2-AA (344)	AF-2 (342)	2-AA (1196)	AF-2 (413)	2-AA (354)	9-AA (709)	2-AA (214)

Mutagenicity in Bacterial Test ; **Negative**

IARC Evaluation ; not yet cited

Experimental Data - 2

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	(117)	(143)	(23)	(16)	(18)	(28)	(15)	(21)	(7)	(8)
	133	142								
	111	141								
0.610	(122)	(142)								
	126	155								
	122	152								
1.22	(124)	(154)								
	135	131	32	14	24	30	10	17	7	5
	141	131	30	6	18	23	15	18	2	6
2.44	(138)	(131)	(31)	(10)	(21)	(27)	(13)	(18)	(5)	(6)
	137	158	24	18	26	29	15	26	5	7
	131	129	26	16	20	24	13	16	7	5
4.88	(134)	(144)	(25)	(17)	(23)	(27)	(14)	(21)	(6)	(6)
	143	121	31	15	28	28	18	21	2	10
	133	138	29	11	29	28	11	21	3	16
9.77	(138)	(130)	(30)	(13)	(29)	(28)	(15)	(21)	(3)	(13)
	109	129	17	8	22	32	13	29	6	2
	142	144	21	18	31	29	10	21	6	5
19.5	(126)	(137)	(19)	(13)	(27)	(31)	(12)	(25)	(6)	(4)
	129*	111	18	18	16	31	21*	21	5	6
	124*	137	16	16	26	30	13*	22	3	10
39.1	(127*)	(124)	(17)	(17)	(21)	(31)	(17*)	(22)	(4)	(8)
	123*	131*	0*	23*	21*	23	0*	29*	0*	7
	109*	158*	0*	14*	13*	18	0*	21*	0*	5
78.1	(116*)	(145*)	(0*)	(19*)	(17*)	(21)	(0*)	(25*)	(0*)	(6)
	75*	86*	0*	0*	0*	0*	0*	0*	0*	0*
	82*	107*	0*	0*	0*	0*	0*	0*	0*	0*
156	(79*)	(97*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
			0*	0*	0*	0*	0*	0*	0*	0*
			0*	0*	0*	0*	0*	0*	0*	0*
313			(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
Judgement	-	-	-	-	-	-	-	-	-	-
Specific Mutagenicity										
Positive Control	AF-2 (933)	2-AA (1533)	NaN ₃ (500)	2-AA (360)	AF-2 (293)	2-AA (1122)	AF-2 (404)	2-AA (328)	9-AA (873)	2-AA (217)

Experimental Data - 3 (B9409-2/3)

Conc. µg/plate	Number of Revertants/plate	
	Base-substitution	
	S9-	S9+
DMSO	(126)	(144)
	128	141
	136	142
0.610	(132)	(142)
	137	156
	121	151
1.22	(129)	(154)
	136	127
	123	149
2.44	(130)	(138)
	120	135
	141	148
4.88	(131)	(142)
	116	152
	119	116
9.77	(118)	(134)
	135	133
	139	137
19.5	(137)	(135)
	135*	119
	129*	143
39.1	(132*)	(131)
	130*	106*
	131*	133*
78.1	(131*)	(120*)
	47*	119*
	64*	113*
156	(56*)	(116*)
Judgement	-	-
Specific Mutagenicity		
Positive Control	AF-2 (799)	2-AA (1338)

Experimental Data - 4

Conc. µg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2uvrA/pKM101	
	S9-	S9+	S9-	S9+	S9-	S9+
DMSO	(324)	(414)	(332)	(453)	(45)	(79)
	305	440	344	456	40	79
	280	449	353	430	41	89
0.0763	(293)	(445)	(349)	(443)	(41)	(84)
	285	395	360	445	60	75
	320	447	374	455	59	85
0.305	(303)	(421)	(367)	(450)	(60)	(80)
	384	418	361	406	52	87
	350	390	366	461	49	83
1.22	(367)	(404)	(364)	(434)	(51)	(85)
	348	411	346	422	63	97
	342	419	328	433	43	93
4.88	(345)	(415)	(337)	(428)	(53)	(95)
	305	417	341	404	49	81
	309	418	328	417	57	78
19.5	(307)	(418)	(335)	(411)	(53)	(80)
	297	438	350	388	49	93
	319	347	388	383	48	87
78.1	(308)	(393)	(369)	(386)	(49)	(90)
	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*
313	(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*
5000	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
Judgement	-	-	-	-	-	-
Specific Mutagenicity						
Positive Control	BLM (1015)	2-AA (1794)	PA (2399)	2-AA (1455)	AF-2 (1218)	2-AA (1082)

Experimental Data - 5

(B9409-3/3)

Conc. µg/plate	Number of Revertants/plate					
	Base-substitution					
	TA102		TA104		WP2uvrA/pKM101	
	S9-	S9+	S9-	S9+	S9-	S9+
DMSO	(319)	(411)	(358)	(465)	(74)	(120)
	311	380	295	394	57	102
	290	377	304	408	59	94
4.88	(301)	(379)	(300)	(401)	(58)	(98)
	280	407	354	418	64	100
	292	390	348	390	63	97
9.77	(286)	(399)	(351)	(404)	(64)	(99)
	309	362	305	389	57	94
	292	300	303	334	49	90
19.5	(301)	(331)	(304)	(362)	(53)	(92)
	293	389	305	399	55	104
	291	371	288	411	51	86
39.1	(292)	(380)	(297)	(405)	(53)	(95)
	291	417	312	401	66	99
	236	370	273	390	68	120
78.1	(264)	(394)	(293)	(396)	(67)	(110)
	159*	293	273*	338	31*	78
	167*	258	265*	331	38*	76
156	(163*)	(276)	(269*)	(335)	(35*)	(77)
	0*	0*	0*	0*	0*	0*
	0*	0*	0*	0*	0*	0*
313	(0*)	(0*)	(0*)	(0*)	(0*)	(0*)
Judgement	-	-	-	-	-	-
Specific Mutagenicity						
Positive Control	BLM (1018)	2-AA (2656)	PA (2575)	2-AA (1486)	AF-2 (1793)	2-AA (1267)