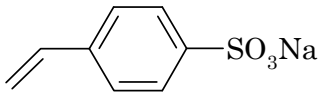
4-Vinylbenzenesulfonic acid sodium salt (4-ﾋﾞﾆﾙﾍﾞﾝｾﾞﾝｽﾙﾎﾝ酸ﾅﾄﾘｳﾑ)

Chemical Name ; 4-Vinylbenzenesulfonic acid sodium salt
Synoym ; Sodium 4-vinylbenzenesulphonate
p-Stylenesulfonic acid sodium salt
4-Sthylenesulfonic acid sodium salt
p-ｽﾁﾚﾝｽﾙﾎﾝ酸ﾅﾄﾘｳﾑ
Molecular Weight ; 206.19
Melting Point ; ≧300℃[Aldrich]
Boiling Point ; －
Flashing Point ; －
Molecular Formular; $C_8H_7NaO_3S$

Chemical Structure;



CAS No. ; 2695-37-6
MITI No. ; (3)-1903, (3)-1948
ML No. ; －
Specified Chemical Substances; －

Source of Substance; Wako Pure Chemical Industries Ltd.
Lot No. ; KLM4046
Purity ; 88.7%

Vehicle ; Distilled H_2O

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*/pKM101		TA98		TA1537	
	S9－	S9＋	S9－	S9＋	S9－	S9＋	S9－	S9＋	S9－	S9＋
H_2O	(121)	(129)	(9)	(9)	(65)	(103)	(14)	(25)	(6)	(13)
1 .22	112 104 (108)	89 117 (103)	8 8 (8)	10 5 (8)	60 55 (58)	99 87 (93)	18 7 (13)	20 23 (22)	5 8 (7)	8 7 (8)
4 .88	117 109 (113)	84 116 (100)	8 7 (8)	7 9 (8)	84 61 (73)	87 91 (89)	10 7 (9)	22 17 (20)	10 7 (9)	10 8 (9)
19 .5	112 105 (109)	122 109 (116)	6 11 (9)	6 14 (10)	62 75 (69)	93 93 (93)	15 23 (19)	23 17 (20)	11 7 (9)	6 7 (7)
78 .1	133 98 (116)	114 106 (110)	8 10 (9)	9 16 (13)	72 55 (64)	109 91 (100)	13 13 (13)	24 17 (21)	6 5 (6)	14 11 (13)
313	111 122 (117)	120 142 (131)	11 10 (11)	8 7 (8)	66 78 (72)	113 108 (111)	23 17 (20)	22 17 (20)	14 14 (14)	7 6 (7)
1250	105 117 (111)	123 126 (125)	11 10 (11)	7 8 (8)	63 79 (71)	96 105 (101)	15 16 (16)	21 18 (20)	9 7 (8)	7 13 (10)
5000	119 129 (124)	106 113 (110)	7 17 (12)	8 14 (11)	55 69 (62)	84 92 (88)	16 11 (14)	14 23 (19)	10 5 (8)	11 3 (7)
Judgement	－	－	－	－	－	－	－	－	－	－
Specific Mutagenicity										
Positive Control	AF-2 (694)	2-AA (1093)	NaN_3 (250)	2-AA (210)	AF-2 (1344)	2-AA (696)	AF-2 (367)	2-AA (322)	9-AA (270)	2-AA (159)

Experimental Data-2

Conc. µg/plate	Number of Revertants/plate									
	Base-substitution						Frame-shift			
	TA100		TA1535		WP2*uvrA*/pKM101		TA98		TA1537	
	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+	S9−	S9+
H_2O	(94)	(114)	(11)	(7)	(61)	(96)	(18)	(22)	(7)	(10)
78 .1	( )	( )	( )	( )	( )	( )	( )	( )	6 5 (6)	( )
156	( )	( )	( )	( )	( )	( )	( )	( )	7 3 (5)	( )
313	90 107 (99)	111 114 (113)	11 6 (9)	9 10 (10)	63 64 (64)	86 86 (86)	15 17 (16)	31 29 (30)	7 8 (8)	6 5 (6)
625	89 112 (101)	107 126 (117)	6 7 (7)	9 11 (10)	44 55 (50)	101 87 (94)	22 21 (22)	16 21 (19)	5 3 (4)	5 6 (6)
1250	104 89 (97)	98 104 (101)	10 9 (10)	7 8 (8)	64 53 (59)	92 86 (89)	10 17 (14)	25 18 (22)	5 7 (6)	11 11 (11)
2500	111 99 (105)	113 100 (107)	8 13 (11)	10 9 (10)	76 66 (71)	101 96 (99)	15 9 (12)	28 32 (30)	9 7 (8)	5 8 (7)
5000	108 98 (103)	111 138 (125)	7 11 (9)	9 2 (6)	60 53 (57)	81 99 (90)	13 13 (13)	21 18 (20)	5 9 (7)	8 6 (7)
	−	−	−	−	−	−	−	−	−	−
Specific Mutagenicity										
Positive Control	AF-2 (645)	2-AA (948)	NaN_3 (299)	2-AA (215)	AF-2 (1313)	2-AA (732)	AF-2 (429)	2-AA (395)	9-AA (464)	2-AA (162)

Experimental Data-3 (B0402-2/2)

Conc. µg/plate	Number of Revertants/plate
	Frame-shift
	TA1537
	S9−
H_2O	(6)
78 .1	5 7 (6)
156	5 5 (5)
313	8 6 (7)
625	3 3 (3)
1250	11 8 (10)
2500	7 6 (7)
5000	9 5 (7)
Judgement	−
Specific Mutagenicity	
Positive Control	9-AA (444)