Diallyldimethylammonium chloride
(ジアリルジメチルアンモニウムクロリド)

Experimental Data-1

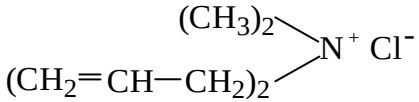
(B9808-1/2)

Chemical Name ; Diallyldimethylammonium chloride

; *N,N*-Dimethyl-*N*-2-propenyl-2-propene-1-ammonium chloride

Molecular Weight ; 161.68
Melting Point ; −
Boiling Point ; −
Flashing Point ; NONE[Aldrich]
Molecular Formula ; $C_8H_{16}ClN$

Chemical Structure



CAS No. ; 7398-69-8
MITI No. ; (2)-3265
ML No. ; 2-(2)-29
Specified Chemical Substances ; −

Source of Substance; Tokyo Kasei Kogyo Co., Ltd.
Lot No. ; FAX01
Purity ; 60% water solution

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*uvr*A/pKM101 | | TA98 | | TA1537 | |
| $H_2O$ | S9− | S9+ | S9− | S9+ | S9− | S9+ | S9− | S9+ | S9− | S9+ |
| | ( 134 ) | ( 122 ) | ( 9 ) | ( 8 ) | ( 59 ) | ( 80 ) | ( 12 ) | ( 20 ) | ( 7 ) | ( 10 ) |
| | 124 | 128 | 7 | 11 | 32 | 82 | 11 | 15 | 3 | 8 |
| | 150 | 141 | 7 | 7 | 51 | 86 | 9 | 24 | 5 | 7 |
| 1 .22 | ( 137 ) | ( 135 ) | ( 7 ) | ( 9 ) | ( 42 ) | ( 84 ) | ( 10 ) | ( 20 ) | ( 4 ) | ( 8 ) |
| | 124 | 135 | 6 | 8 | 59 | 96 | 20 | 26 | 5 | 10 |
| | 135 | 136 | 10 | 13 | 54 | 83 | 13 | 17 | 5 | 5 |
| 4 .88 | ( 130 ) | ( 136 ) | ( 8 ) | ( 11 ) | ( 57 ) | ( 90 ) | ( 17 ) | ( 22 ) | ( 5 ) | ( 8 ) |
| | 160 | 135 | 5 | 11 | 70 | 99 | 13 | 30 | 5 | 5 |
| | 142 | 121 | 18 | 9 | 61 | 86 | 13 | 20 | 6 | 7 |
| 19 .5 | ( 151 ) | ( 128 ) | ( 12 ) | ( 10 ) | ( 66 ) | ( 93 ) | ( 13 ) | ( 25 ) | ( 6 ) | ( 6 ) |
| | 128 | 124 | 13 | 11 | 56 | 92 | 10 | 20 | 5 | 9 |
| | 138 | 124 | 15 | 7 | 49 | 89 | 17 | 15 | 6 | 10 |
| 78 .1 | ( 133 ) | ( 124 ) | ( 14 ) | ( 9 ) | ( 53 ) | ( 91 ) | ( 14 ) | ( 18 ) | ( 6 ) | ( 10 ) |
| | 137 | 162 | 11 | 3 | 67 | 82 | 11 | 11 | 2 | 8 |
| | 135 | 126 | 8 | 7 | 66 | 69 | 22 | 20 | 3 | 13 |
| 313 | ( 136 ) | ( 144 ) | ( 10 ) | ( 5 ) | ( 67 ) | ( 76 ) | ( 17 ) | ( 16 ) | ( 3 ) | ( 11 ) |
| | 122 | 102 | 10 | 9 | 84 | 90 | 15 | 15 | 7 | 3 |
| | 130 | 120 | 9 | 8 | 54 | 75 | 16 | 25 | 6 | 5 |
| 1250 | ( 126 ) | ( 111 ) | ( 10 ) | ( 9 ) | ( 69 ) | ( 83 ) | ( 16 ) | ( 20 ) | ( 7 ) | ( 4 ) |
| | 100 * | 111 | 2 * | 8 | 38 * | 78 * | 13 * | 21 | 2 * | 13 |
| | 113 * | 89 | 6 * | 11 | 32 * | 98 * | 13 * | 20 | 3 * | 7 |
| 5000 | ( 107 *) | ( 100 ) | ( 4 *) | ( 10 ) | ( 35 *) | ( 88 *) | ( 13 *) | ( 21 ) | ( 3 *) | ( 10 ) |
| Judgement | − | − | − | − | − | − | − | − | − | − |
| Specific Mutagenicity | | | | | | | | | | |
| Positive Control | AF-2 | 2-AA | $NaN_3$ | 2-AA | AF-2 | 2-AA | AF-2 | 2-AA | 9-AA | 2-AA |
| | ( 647 ) | ( 1073 ) | ( 444 ) | ( 267 ) | ( 780 ) | ( 738 ) | ( 429 ) | ( 405 ) | ( 451 ) | ( 195 ) |

* Growth inhibitation was observed.

Experimental Data-2

| Conc. μg/plate | Number of Revertants/plate | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | Base-substitution | | | | | | Frame-shift | | | |
| | TA100 | | TA1535 | | WP2*uvr*A/pKM101 | | TA98 | | TA1537 | |
| $H_2O$ | S9− | S9+ | S9− | S9+ | S9− | S9+ | S9− | S9+ | S9− | S9+ |
| | ( 120 ) | ( 144 ) | ( 8 ) | ( 9 ) | ( 66 ) | | ( 19 ) | ( 29 ) | ( 6 ) | ( 8 ) |
| | 146 | | 5 | | 47 | | 15 | | 6 | |
| | 149 | | 6 | | 49 | | 18 | | 7 | |
| 78 .1 | ( 148 ) | | ( 6 ) | | ( 48 ) | | ( 17 ) | | ( 7 ) | |
| | 142 | | 10 | | 79 | | 21 | | 3 | |
| | 155 | | 8 | | 76 | | 21 | | 7 | |
| 156 | ( 149 ) | | ( 9 ) | | ( 78 ) | | ( 21 ) | | ( 5 ) | |
| | 150 | 153 | 6 | 11 | 70 | | 22 | 32 | 3 | 9 |
| | 130 | 131 | 7 | 7 | 64 | | 17 | 20 | 3 | 9 |
| 313 | ( 140 ) | ( 142 ) | ( 7 ) | ( 9 ) | ( 67 ) | | ( 20 ) | ( 26 ) | ( 3 ) | ( 9 ) |
| | 143 | 130 | 10 | 11 | 67 | | 18 | 24 | 5 | 5 |
| | 142 | 138 | 6 | 11 | 54 | | 18 | 25 | 7 | 7 |
| 625 | ( 143 ) | ( 134 ) | ( 8 ) | ( 11 ) | ( 61 ) | | ( 18 ) | ( 25 ) | ( 6 ) | ( 6 ) |
| | 148 | 117 | 7 | 6 | 71 | | 20 | 18 | 6 | 7 |
| | 122 | 136 | 3 | 10 | 74 | | 23 | 21 | 7 | 8 |
| 1250 | ( 135 ) | ( 127 ) | ( 5 ) | ( 8 ) | ( 73 ) | | ( 22 ) | ( 20 ) | ( 7 ) | ( 8 ) |
| | 150 * | 136 | 9 * | 7 | 75 | | 18 | 21 | 2 * | 10 |
| | 120 * | 148 | 3 * | 7 | 62 | | 15 | 28 | 3 * | 10 |
| 2500 | ( 135 *) | ( 142 ) | ( 6 *) | ( 7 ) | ( 69 ) | | ( 17 ) | ( 25 ) | ( 3 *) | ( 10 ) |
| | 101 * | 137 | 5 * | 8 | 33 * | | 8 * | 25 | 2 * | 6 |
| | 108 * | 117 | 6 * | 5 | 48 * | | 10 * | 24 | 1 * | 14 |
| 5000 | ( 105 *) | ( 127 ) | ( 6 *) | ( 7 ) | ( 41 *) | | ( 9 *) | ( 25 ) | ( 2 *) | ( 10 ) |
| Judgement | − | − | − | − | − | | − | − | − | − |
| Specific Mutagenicity | | | | | | | | | | |
| Positive Control | AF-2 ( 563 ) | 2-AA ( 1102 ) | $NaN_3$ ( 429 ) | 2-AA ( 254 ) | AF-2 ( 587 ) | | AF-2 ( 504 ) | 2-AA ( 391 ) | 9-AA ( 397 ) | 2-AA ( 151 ) |

Experimental Data-3

| Conc. μg/plate | Number of Revertants/plate | |
|---|---|---|
| | Base-substitution | |
| | WP2*uvr*A/pKM101 | |
| $H_2O$ | S9− | S9+ |
| | ( 42 ) | ( 70 ) |
| | | 54 |
| | | 62 |
| 78 .1 | | ( 58 ) |
| | | 55 |
| | | 85 |
| 156 | | ( 70 ) |
| | | 66 |
| | | 81 |
| 313 | | ( 74 ) |
| | | 61 |
| | | 91 |
| 625 | | ( 76 ) |
| | | 66 |
| | | 64 |
| 1250 | | ( 65 ) |
| | | 68 |
| | | 54 |
| 2500 | | ( 61 ) |
| | | 54 * |
| | | 57 * |
| 5000 | | ( 56 *) |
| Judgement | | − |
| Specific Mutagenicity | | |
| Positive Control | AF-2 ( 675 ) | 2-AA ( 802 ) |