Chemical Name ; 3-Methoxybutyl acetate

Synonym ; 3-Methoxy-1-butyl-acetate
Acetic acid 3-methoxybutyl ester
3−ﾒﾄｷｼﾌﾞﾁﾙｱｾﾀｰﾄ

Molecular Weight ; 146.19
Melting Point ; −
Boiling Point ; 170-172℃[CHCD]
Flashing Point ; −
Molecular Formula ; $C_7H_{14}O_3$

Chemical Structure

$CH_3COO(CH_2)_2CH(OCH_3)CH_3$

CAS No. ; 4435-53-4
MITI No. ; (2)-739
ML No. ; −
Specified Chemical Substances ; −

Source of Substance; Tokyo Kasei Kogyo Co., Ltd.
Lot No. ; GB01
Purity ; >99%

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+ |
| | ( 132 ) | ( 139 ) | ( 8 ) | ( 10 ) | ( 42 ) | ( 75 ) | ( 15 ) | ( 21 ) | ( 6 ) | ( 8 ) |
| | 119 | 164 | 8 | 9 | 39 | 69 | 10 | 26 | 6 | 9 |
| | 126 | 146 | 5 | 13 | 48 | 82 | 20 | 28 | 6 | 13 |
| 1 .22 | ( 123 ) | ( 155 ) | ( 7 ) | ( 11 ) | ( 44 ) | ( 76 ) | ( 15 ) | ( 27 ) | ( 6 ) | ( 11 ) |
| | 130 | 146 | 10 | 9 | 46 | 78 | 14 | 24 | 5 | 8 |
| | 130 | 126 | 9 | 11 | 55 | 79 | 18 | 16 | 5 | 5 |
| 4 .88 | ( 130 ) | ( 136 ) | ( 10 ) | ( 10 ) | ( 51 ) | ( 79 ) | ( 16 ) | ( 20 ) | ( 5 ) | ( 7 ) |
| | 120 | 152 | 7 | 5 | 45 | 86 | 14 | 20 | 3 | 6 |
| | 148 | 127 | 8 | 8 | 56 | 67 | 18 | 21 | 10 | 5 |
| 19 .5 | ( 134 ) | ( 140 ) | ( 8 ) | ( 7 ) | ( 51 ) | ( 77 ) | ( 16 ) | ( 21 ) | ( 7 ) | ( 6 ) |
| | 120 | 133 | 8 | 9 | 31 | 81 | 13 | 26 | 5 | 10 |
| | 115 | 141 | 9 | 13 | 40 | 79 | 11 | 17 | 6 | 6 |
| 78 .1 | ( 118 ) | ( 137 ) | ( 9 ) | ( 11 ) | ( 36 ) | ( 80 ) | ( 12 ) | ( 22 ) | ( 6 ) | ( 8 ) |
| | 130 | 128 | 9 | 9 | 40 | 85 | 14 | 23 | 3 | 6 |
| | 141 | 137 | 7 | 11 | 44 | 84 | 17 | 25 | 3 | 7 |
| 313 | ( 136 ) | ( 133 ) | ( 8 ) | ( 10 ) | ( 42 ) | ( 85 ) | ( 16 ) | ( 24 ) | ( 3 ) | ( 7 ) |
| | 156 | 149 | 3 | 11 | 46 | 76 | 17 | 22 | 6 | 11 |
| | 134 | 128 | 10 | 13 | 40 | 75 | 17 | 25 | 5 | 10 |
| 1250 | ( 145 ) | ( 139 ) | ( 7 ) | ( 12 ) | ( 43 ) | ( 76 ) | ( 17 ) | ( 24 ) | ( 6 ) | ( 11 ) |
| | 120 | 122 | 9 | 10 | 43 | 78 | 15 | 20 | 5 | 9 |
| | 122 | 136 | 11 | 7 | 37 | 57 | 15 | 25 | 6 | 6 |
| 5000 | ( 121 ) | ( 129 ) | ( 10 ) | ( 9 ) | ( 40 ) | ( 68 ) | ( 15 ) | ( 23 ) | ( 6 ) | ( 8 ) |
| Judgement | − | − | − | − | − | − | − | − | − | − |
| Specific Mutagenicity | | | | | | | | | | |
| Positive Control | AF-2 ( 806 ) | 2-AA ( 1567 ) | $NaN_3$ ( 383 ) | 2-AA ( 356 ) | AF-2 ( 1958 ) | 2-AA ( 1080 ) | AF-2 ( 465 ) | 2-AA ( 464 ) | 9-AA ( 794 ) | 2-AA ( 250 ) |

| 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+ |
| | ( 139 ) | ( 154 ) | ( 7 ) | ( 12 ) | ( 32 ) | ( 56 ) | ( 17 ) | ( 26 ) | ( 6 ) | ( 7 ) |
| | 137 | 157 | 3 | 10 | 26 | 57 | 16 | 30 | 5 | 8 |
| | 148 | 163 | 5 | 11 | 32 | 64 | 22 | 24 | 3 | 10 |
| 313 | ( 143 ) | ( 160 ) | ( 4 ) | ( 11 ) | ( 29 ) | ( 61 ) | ( 19 ) | ( 27 ) | ( 4 ) | ( 9 ) |
| | 136 | 181 | 7 | 8 | 39 | 40 | 20 | 32 | 7 | 8 |
| | 153 | 143 | 8 | 13 | 47 | 72 | 26 | 31 | 3 | 5 |
| 625 | ( 145 ) | ( 162 ) | ( 8 ) | ( 11 ) | ( 43 ) | ( 56 ) | ( 23 ) | ( 32 ) | ( 5 ) | ( 7 ) |
| | 159 | 174 | 7 | 14 | 38 | 64 | 22 | 36 | 8 | 5 |
| | 131 | 171 | 5 | 9 | 29 | 57 | 15 | 29 | 5 | 9 |
| 1250 | ( 145 ) | ( 173 ) | ( 6 ) | ( 12 ) | ( 34 ) | ( 61 ) | ( 19 ) | ( 33 ) | ( 7 ) | ( 7 ) |
| | 134 | 181 | 6 | 14 | 34 | 64 | 29 | 24 | 5 | 7 |
| | 144 | 177 | 7 | 14 | 29 | 66 | 17 | 24 | 5 | 9 |
| 2500 | ( 139 ) | ( 179 ) | ( 7 ) | ( 14 ) | ( 32 ) | ( 65 ) | ( 23 ) | ( 24 ) | ( 5 ) | ( 8 ) |
| | 159 | 148 | 8 | 17 | 33 | 51 | 17 | 28 | 8 | 9 |
| | 135 | 166 | 11 | 11 | 39 | 55 | 18 | 23 | 5 | 9 |
| 5000 | ( 147 ) | ( 157 ) | ( 10 ) | ( 14 ) | ( 36 ) | ( 53 ) | ( 18 ) | ( 26 ) | ( 7 ) | ( 9 ) |
| Judgement | − | − | − | − | − | − | − | − | − | − |
| Specific Mutagenicity | | | | | | | | | | |
| Positive Control | AF-2 ( 655 ) | 2-AA ( 1191 ) | $NaN_3$ ( 429 ) | 2-AA ( 358 ) | AF-2 ( 694 ) | 2-AA ( 842 ) | AF-2 ( 511 ) | 2-AA ( 433 ) | 9-AA ( 632 ) | 2-AA ( 200 ) |