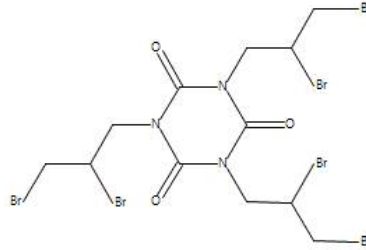**Test Results for Chemical # 1**

1,3,5-tris(2,3-dibromopropyl)-1,3,5-triazinane-2,4,6-trione

Model: GT1_BMUT (Statistical-based Model for Bacterial Mutagenicity by OECD 471 test guidance)

Model Version: 1.8.0.1.11479.500

Tested by CASE Ultra Version: 1.8.0.5

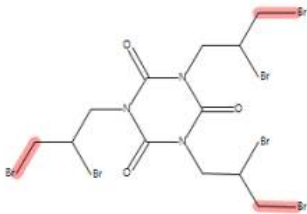|	
Compound Name	1,3,5-tris(2,3-dibromopropyl)-1,3,5-triazinane-2,4 ,6-trione
Registry #	52434-90-9
Molecular Weight	728.694
SMILES Code	BrCC(Br)CN1C(=O)N(CC(Br)CBr)C(=O)N(CC(Br)CBr)C1=O

Test Outcome: POSITIVE
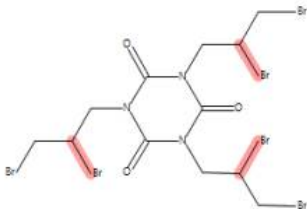
Alert Group #1

Composed of Alert with ID #82

Alert ID 82: `C3H2-Br`

110 out of 127 (86.6%) compounds containing this alert are positive with an average activity of 0.87

Strong Alert: This alert (#82) will increase the probability of being positive to 79.7% if no other alerts are present.

Alert Group #2

Composed of Alert with ID #95

Alert ID 95: `C3H-Br`

66 out of 79 (83.5%) compounds containing this alert are positive with an average activity of 0.84

Strong Alert: This alert (#95) will increase the probability of being positive to 67.9% if no other alerts are present.

Deactivating Features

Two deactivating features were found in the test chemical.

Fragment ID 687: `N3-C2(-N3)=O`
29 out of 78 (37.2%) compounds containing this feature are positive with an average activity of 0.37

Deactivating Potential: This fragment (#687) will decrease the probability of being positive by 1.3% if no other deactivating features are present.

Fragment ID 141: `C3H-C3H2-N3`
115 out of 209 (55.0%) compounds containing this feature are positive with an average activity of 0.55

Deactivating Potential: This fragment (#141) will decrease the probability of being positive by 1.3% if no other deactivating features are present.

QSAR Prediction:

Contribution of Positive Alerts:
Weighted Contribution of Alert ID 82 = QSAR Coeff: 2.666 * Value: 1.000 = 2.666
Weighted Contribution of Alert ID 95 = QSAR Coeff: 2.048 * Value: 1.000 = 2.048
Contribution of Deactivating Features:
Weighted Contribution of Fragment ID 687 = QSAR Coeff: -0.357 * Value: 1.000 = -0.357
Weighted Contribution of Fragment ID 141 = QSAR Coeff: -0.348 * Value: 1.000 = -0.348
QSAR Constant = -1.299

Sum of Factors = 2.666+2.048-0.357-0.348-1.299 = 2.710
Calculated probability using the global QSAR = $1/(1+e^{-1 * 2.710})$ = 0.938 (93.8%)
Baseline probability (calculated using the QSAR constant) = $1/(1+e^{-1 * -1.299})$ = 0.214 (21.4%)

CONCLUSIONS

- The query compound is predicted to be **POSITIVE** in the test using the model GT1_BMUT (Statistical-based Model for Bacterial Mutagenicity by OECD 471 test guidance).

- The QSAR calculated probability is 93.8%.

- The calculated probability is HIGHER than the model's current classification threshold (50.0%) and not within the gray zone.The gray zone for this model is between 40.0% to 60.0%.

Notes: Positive alerts increase, and deactivating features decrease overall probability to be active. For any particular positive alert, +ve modulators increase and -ve modulators decrease alert's effect on the overall calculated probability (if present).