Supporting Information:

Adsorption of dibenzo-*p*-dioxins on the surface of C60 fullerene. The influence of halogenation: calculations and QSPR predictions

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Number of tables: 3

1. Details on materials and methods
   1. Structural descriptors

Calculations of molecular descriptors can be performed based only on chemical formula or on theoretical chemistry methods. Table S1 presents the list of structural descriptors calculated for all 1701 congeners of brominated, chlorinated and bromo-chlorinated dibenzo*-p-*dioxins. Dioxin database was created as a part of bigger Persistent Organic Pollutants database described in our previous study1 All calculations were performed with MOPAC 20072 package with using the increased criteria of precision (PRECISE keyword) with PM6 semi-empirical method. Using structural descriptors for nano-QSPR modeling of sorption potential calculated as an endpoint on DFT level is, as we believe, possible according to the most important conclusions of the latter study3.

Table S1 List of the structural descriptors.

|  |  |  |  |
| --- | --- | --- | --- |
| No. | Symbol | Description | Selected to the QSPR model |
| 1. | #H | The number of hydrogen atoms | YES |
| 2. | #Cl | Number of chlorine atoms | NO |
| 3. | #Br | Number of bromine atoms | NO |
| 4. | nAT | Total number of atoms in a molecule | NO |
| 5. | HOF | Heat of formation | NO |
| 6. | EE | Electronic energy | NO |
| 7. | Core | Core repulsion energy | NO |
| 8. | TE | Total energy of a molecule | YES |
| 9. | HOMO | Energy of the highest occupied molecular orbital | NO |
| 10. | LUMO | Energy of the lowest unoccupied molecular orbital | NO |
| 11. | HOFc | Heat of formation in water | NO |
| 12. | Tec | Total energy in water | NO |
| 13. | SAS | Solvent accessible surface | NO |
| 14. | MV | Molecular volume | NO |
| 15. | MW | Molecular weight | NO |
| 16. | D | Dipole moment | NO |
| 17. | D\_x | X axis dipole moment | YES |
| 18. | D\_y | Y axis dipole moment | YES |
| 19. | D\_z | Z axis dipole moment | NO |
| 20. | q\_min | The lowest negative Mulliken partial charge (q\_min) | NO |
| 21. | q\_max | The highest negative Mulliken partial charge (q\_max) | NO |
| 22. | Ahof | Polarizability derived from the heat of formation (Ahof) | NO |
| 23. | Ad | Polarizability derived from the dipole moment (Ad) | NO |
| 24. | EN | Mulliken electronegativity | NO |
| 25. | Hard | Parr and Pople’s absolute hardness | NO |
| 26. | Shift | Schurmann MO shift alpha | NO |

* 1. Selection of representative subset of dioxins for energy calculations

A subset of 32 representative congeners was selected by using Kennard-Stone algorithm4. As a result we got a subset containing the central object in the data, then furthest object from it, than furthest from selected two and so one. So for energy calculations the outliers and farthest objects situated on the surface of the multidimensional cloud formed by all of the objects (compounds) and objects representatively located inside the cloud were chosen.

* 1. The starting position influence and starting distance verification.

Influence of a starting positions of molecules was verified by Molecular Mechanics calculations. Dioxin and fullerene molecules were built in Avogadro5 software. A Ghemical Force Field was set up with 500 steps and the Steepest Descent algorithm with convergence on 10-7 level. A Ghemical Force Field is a variant of the Tripos-5.2 Force Field. It is implemented to the Avogadro software, and it was successfully used for carbon nanomaterials like graphene and other chemicals calculations in other studies before6, 7.

Calculations for the 2,3,7,8-TCDD@C60 complexes were performed with initial distances between one of the oxygen atoms from the central dioxin ring and the nearest carbon atom in fullerene. All calculations were performed for position 1 described in manuscript and starting distances: 2.5Å, 3Å, 3.5Å, 4Å, 4.5Å and 5Å respectively. For this part, methods based on Density Functional Theory (so called DFT methods) were implemented

* 1. Quantum mechanical calculations

After a literature research, M06-2X DFT method was chosen. It is known to be suitable for nanoparticles calculations, and what is also relevant, weak Van der Waals and stacking interactions between molecules. Truhlar’s hybrid DFT functionals like M05-2X and newer M06-2X, were commonly used in weak interactions modeling, and gave reliable calculation results without the Basis Set Superposition Error (BSSE) corrections, which was proved in previously published studies 8-11.

ONIOM method used in this study allows to model large molecules by defining two or three layers within the structure that are treated at different levels of accuracy. Calibration studies have demonstrated that the resulting predictions are essentially equivalent to those that produced by the high accuracy method alone on the entire molecule. Two layers in the fullerene structure were defined to reduce the computation time in this study. 6-31++g(d,p) basis set was set for high computation layer and 3-21g basis set was used for the lower one (fullerene carbon atoms located on the opposite side from the surface on which the π-π interactions were expected).

1. Details on the QSPR modeling
   1. QSPR details

The usual QSPR procedure involves (i) collection of experimental data/theoretical calculation of data; (ii) calculation of molecular descriptors for all the studied compounds (this part was fulfilled in earlier studies)12; (iii) splitting of the compounds for which experimental/calculated data exist into two sets, a training set (TS) and a validation set (VS); (iv) calibration of the model with the training set; (v) external validation with the validation set; and (vi) if the model passes the validation criteria, prediction of values for new compounds

* 1. OECD principles

The OECD principles for (Q)SAR (Quantitative Structure Activity Relationship) methods assume that correctly developed and validated model should have: (i) a well defined predicted endpoint, (ii) an unambiguous algorithm, (iii)a defined domain of applicability, (iv) appropriate measures of goodness-of-fit, robustness and predictivity and (v) a mechanistic interpretation, if possible

* 1. Splitting data for training and validation set

After the sorption energy calculations, endpoint value, as an extra column was added to the descriptors matrix. Data was sorted by increasing values of calculated sorption energy for each dioxin structure, and split on training (TS) and validation (VS) sets in a way to be ensured that points from a VS are evenly distributed within the range of the calculated energies in the training set. In sorted data set we utilized the following pattern of splitting: TS-TS-**VS**-TS-TS-TS-**VS**-TS-TS-TS-**VS**-(…)-TS-TS-TS-**VS**-TS, called 1:X, (where X=4). It was fitted to data to ensure that the first and the last compound in the data set belongs to TS to avoid errors in external validation. Compounds with assignment to TS and VS can be found in Table S2.

* 1. Preprocessing of data, internal validation, statistical measures of goodness-of-fit and robustness of the QSPR model

The data set was auto-scaled, so the average value was subtracted from the descriptors, and the resultant values divided by the standard deviation to ensure the same scale and range of all variables.

As goodness-of-fit parameters, the determination coefficient R2(1) and the Root mean Square Error of Calibration (RMSEC) (2) were used.

 (1)

 (2)

Where: *yiobs* – the experimental (calculated) value of the property for the *i*th compound; *yi pred* – the predicted value for the *i*th compound;; *ỹobs* – the mean experimental value of the property in the training set; *n* – the number of compounds in the training set.

Internal validation (cross-validation leve-one-out technique, CV LOO) was applied to reduce the probability of model’s overfitting to the training data, and to measure robustness of the model. According to CV LOO algorithm each dioxin congener from training set was removed, one at a time. Thus, 24 reduced models were calculated; each of it was developed with the remaining 23 congeners in TS and used to predict the sorption energy of the congener temporarily removed. The cross-validated correlation coefficient Q2CV (3) and cross-validated Root Mean Square Error of Cross-Validation RMSECV (4) were calculated.

 (3)

 (4)

Where *yi predcv* – is the predicted value for the temporary excluded (cross-validated) *i*th compound.

* 1. External validation and measures of predictive ability

By applying of the model to the validation set (not previously used to develop the model), we confirmed the models’ prediction ability. Predictive ability of the model is described by the externally validated determination coefficient Q2Ext (5) and the Root Mean Square Error of Prediction RMSEP (6)

 (5)

 (6)

Where: *yjobs* – the experimental (observed) value of the property for the *j*th compound; *yjpred*– the predicted value for *j*th compound; *ỹobs*  – the mean experimental value of the property in the validation set; *k* – the number of compounds in the validation set.

QSPR model equation and values calculated by using equations 1-6 are presented below:

ΔEads [kcal/mol] = 7.37 **#H** -6.76 **TE** -0.11 **D\_x** - 0.07 **D\_y**

R2= 0.998 Q2CV= 0.987 Q2Ext = 0.956 (7)

RMSEC=1.18 RMSECV= 1.468 RMSEP= 2.285

2.4 Applicability domain of the model.

Insubria plot presented on Figure S1 gives the full information about all congeners from training, validation and prediction sets in the space called applicability domain of the QSPR model. It can be noticed that only few from 1701 congeners (from prediction set) have leverage values higher that the critical h\*=0.625, what gives the information that those particular predictions are based on extrapolation of a model and are less reliable. The leverage (*hi*) is defined by:

 *i*=(1,……..,n) (8)

where xi is the vector of descriptors calculated for the considered compound and X is the matrix of descriptors calculated for the training set.

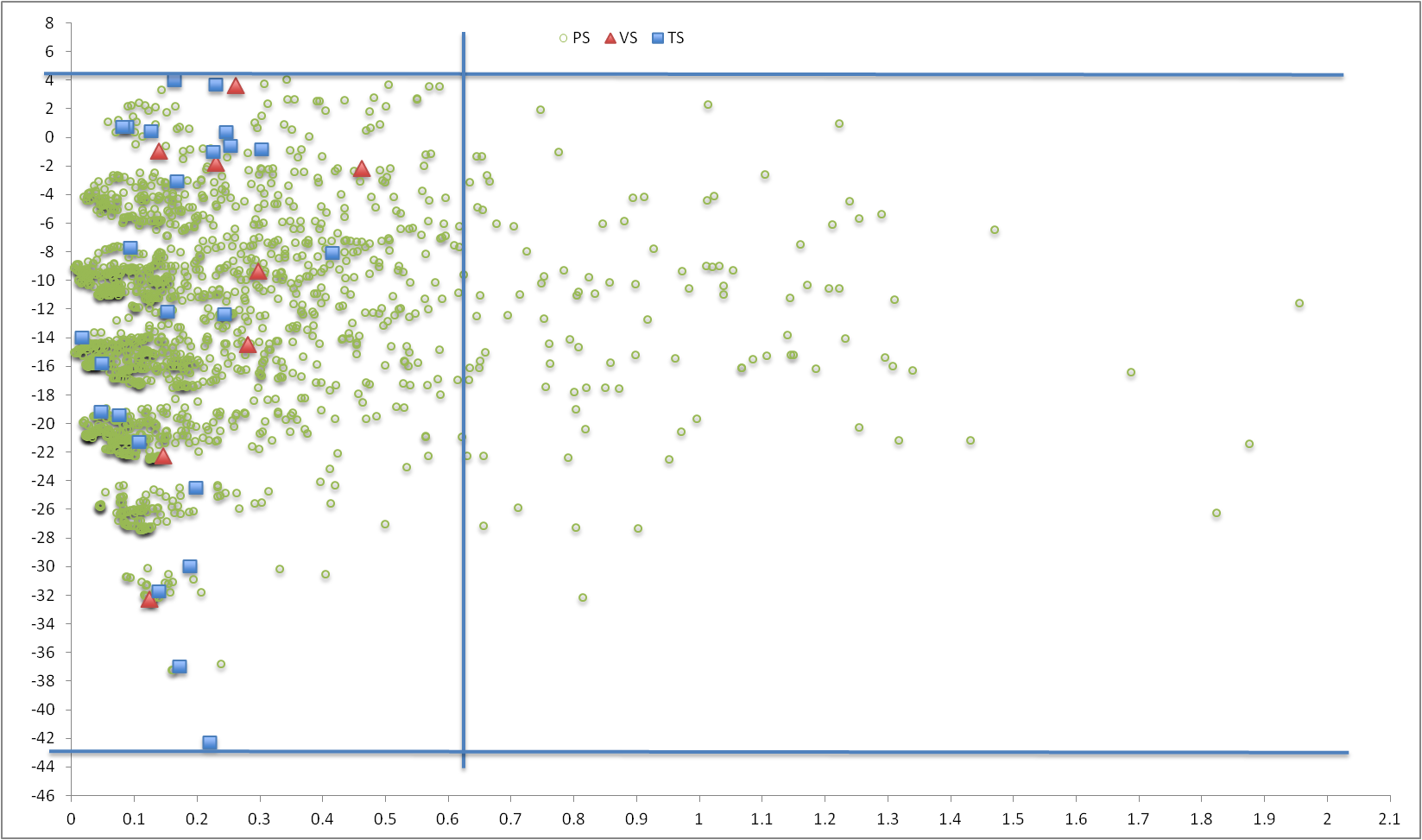


Figure S1. The Insubria Plot, with yobs minimum and maximum values and the h\*=0.625 marked by blue lines.

Table S2. List of congeners selected to training and validation sets (TS/VS) with descriptors used in nano-QSPR model (#H - number of H atoms in the molecule, TE - total energy molecule D\_x, D\_y - dipol moments along X and Y axis). ΔE Calc/Pred Energies calculated/predicted [kcal/mol]

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **IUPAC name** | **#H** | **TE** | **D\_x** | **D\_y** | **ΔE Calc.** | **ΔE Pred.** | | **Training/ Validation** |
| 1,2,3,4,6,7,8,9-octobromodibenzo*-p-*dioxin | 0 | -3874.06 | 0.00 | 0.00 | -41.69 | -42.27 | TS | |
| 1,2,3,4,6,7,8-heptabromodibenzo*-p-*dioxin | 1 | -3659.79 | 0.50 | -0.02 | -35.29 | -36.95 | TS | |
| 1,2,3,7,8,9-hexabromodibenzo*-p-*dioxin | 2 | -3445.52 | -1.13 | 0.06 | -31.47 | -29.98 | TS | |
| 1,2,3,4,6,9-hexabromo-7-chlorodibenzo*-p-*dioxin | 1 | -3686.27 | -0.04 | 0.01 | -31.27 | -31.74 | TS | |
| 1,2,4,7,8-pentabromodibenzo*-p-*dioxin | 3 | -3231.25 | -0.02 | -0.02 | -24.35 | -24.47 | TS | |
| 1,4,6,9-tetrabromodibenzo*-p-*dioxin | 4 | -3016.81 | 0.00 | 0.01 | -22.57 | -19.41 | TS | |
| 1,3,7,9-tetrabromo-4,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.48 | 0.82 | -0.04 | -22.49 | -21.29 | TS | |
| 2,3,7,8-tetrabromodibenzo*-p-*dioxin | 4 | -3016.97 | 0.00 | 0.00 | -17.74 | -19.17 | TS | |
| 1,3,8-tribromo-2,6,7-trichlorodibenzo*-p-*dioxin | 2 | -3524.89 | 0.10 | -0.01 | -15.46 | -15.81 | TS | |
| 1,3,9-tribromo-7-chlorodibenzo*-p-*dioxin | 4 | -3043.52 | -0.45 | 0.03 | -14.67 | -13.96 | TS | |
| 1,7-dibromo-2,3,4,6,8,9-hexachlorodibenzo*-p-*dioxin | 0 | -4033.02 | 0.03 | 0.00 | -13.64 | -12.35 | TS | |
| 2,8-dibromo-1,3,4,6,7-pentachlorodibenzo*-p-*dioxin | 1 | -3792.24 | 0.66 | -0.02 | -12.57 | -12.18 | TS | |
| 2,8-dibromo-1,3,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.61 | -2.44 | 0.11 | -6.81 | -8.07 | TS | |
| 2,7-dibromodibenzo*-p-*dioxin | 6 | -2588.22 | 0.00 | 0.00 | -6.12 | -7.70 | TS | |
| 1-bromo-4,8-dichlorodibenzo*-p-*dioxin | 5 | -2855.65 | -0.14 | -0.01 | -3.00 | -3.04 | TS | |
| 2-bromodibenzo*-p-*dioxin | 7 | -2373.74 | -1.55 | 0.08 | -1.38 | -0.99 | TS | |
| 1,2,3,4,7-pentachlorodibenzo*-p-*dioxin | 3 | -3363.81 | 0.01 | 0.03 | -1.27 | -0.83 | TS | |
| 1,2,3,4,6,9-hexachlorodibenzo*-p-*dioxin | 2 | -3604.65 | -1.06 | 0.07 | -0.48 | -0.58 | TS | |
| 1,4,6,9-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.04 | 0.00 | 0.00 | 0.29 | 0.75 | TS | |
| 2,3,7,8-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.10 | 0.00 | 0.00 | 0.96 | 0.73 | TS | |
| 1,4,6-trichlorodibenzo*-p-*dioxin | 5 | -2882.11 | 0.79 | -0.02 | 1.27 | 0.40 | TS | |
| 1,2,4,6,9-pentachlorodibenzo*-p-*dioxin | 3 | -3363.91 | -1.03 | 0.06 | 2.20 | 0.42 | TS | |
| 1-chlorodibenzo*-p-*dioxin | 7 | -2400.22 | -1.31 | 0.06 | 2.33 | 3.98 | TS | |
| dibenzo*-p-*dioxin | 8 | -2159.25 | 0.00 | 0.00 | 4.40 | 3.72 | TS | |
| 1,2,3,4,6,8-hexabromo-7,9-dichlorodibenzo*-p-*dioxin | 0 | -3926.92 | -0.07 | 0.01 | -33.19 | -32.25 | VS | |
| 1,2,3,6-tetrabromo-4,7,8,9-tetrachlorodibenzo*-p-*dioxin | 0 | -3980.04 | -0.01 | 0.00 | -22.57 | -22.25 | VS | |
| 1,2,4-tribromo-7,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.32 | -0.01 | -0.02 | -15.68 | -14.44 | VS | |
| 1,3-dibromo-2,4,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.37 | -1.75 | 0.08 | -13.58 | -9.35 | VS | |
| 2-bromo-1,8,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.36 | -2.63 | 0.12 | -5.66 | -2.15 | VS | |
| 1,2,3,4,6,8-hexachlorodibenzo*-p-*dioxin | 2 | -3604.73 | -0.21 | 0.02 | -0.62 | -0.94 | VS | |
| 1,2,3,4,6,7,9-heptachlorodibenzo*-p-*dioxin | 1 | -3845.51 | -0.04 | 0.01 | 1.19 | -1.79 | VS | |
| 1,9-dichlorodibenzo*-p-*dioxin | 6 | -2641.17 | -2.08 | 0.10 | 3.45 | 3.62 | VS | |

Table S3 Sorption energy values (ΔEPred [kcal/mol]) predicted for congeners in prediction set. #H – the number of hydrogen atoms in the structure, TE-Total Energy of particular dioxin structure, D\_x and D\_y – dipole moments along X and Y axis respectively

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| IUPAC name | #H | TE | D\_x | D\_y | ΔE Pred |
| 2-chlorodibenzo*-p-*dioxin | 7 | -2400.308 | -1.581 | 0.089 | 3.750 |
| 1-bromodibenzo*-p-*dioxin | 7 | -2373.660 | -1.281 | 0.071 | -1.373 |
| 1,2-dichlorodibenzo*-p-*dioxin | 6 | -2641.117 | -2.380 | 0.108 | 4.037 |
| 1,3-dichlorodibenzo*-p-*dioxin | 6 | -2641.250 | -1.379 | 0.088 | 2.647 |
| 1,4-dichlorodibenzo*-p-*dioxin | 6 | -2641.164 | -0.400 | 0.034 | 2.142 |
| 1,6-dichlorodibenzo*-p-*dioxin | 6 | -2641.182 | 0.000 | 0.003 | 2.177 |
| 1,7-dichlorodibenzo*-p-*dioxin | 6 | -2641.267 | 0.279 | -0.038 | 2.719 |
| 1,8-dichlorodibenzo*-p-*dioxin | 6 | -2641.266 | -1.053 | 0.023 | 3.708 |
| 2,3-dichlorodibenzo*-p-*dioxin | 6 | -2641.193 | -1.479 | 0.096 | 2.622 |
| 2,7-dichlorodibenzo*-p-*dioxin | 6 | -2641.355 | 0.000 | 0.001 | 2.261 |
| 2,8-dichlorodibenzo*-p-*dioxin | 6 | -2641.353 | -1.334 | 0.058 | 3.358 |
| 1-bromo-2-chlorodibenzo*-p-*dioxin | 6 | -2614.529 | -2.322 | 0.100 | -0.867 |
| 1-bromo-3-chlorodibenzo*-p-*dioxin | 6 | -2614.685 | -1.330 | 0.096 | -2.650 |
| 1-bromo-4-chlorodibenzo*-p-*dioxin | 6 | -2614.607 | -0.365 | 0.036 | -2.972 |
| 1-bromo-6-chlorodibenzo*-p-*dioxin | 6 | -2614.622 | 0.038 | 0.014 | -3.176 |
| 1-bromo-7-chlorodibenzo*-p-*dioxin | 6 | -2614.708 | 0.310 | -0.038 | -2.335 |
| 1-bromo-8-chlorodibenzo*-p-*dioxin | 6 | -2614.706 | -1.024 | 0.025 | -1.394 |
| 1-bromo-9-chlorodibenzo*-p-*dioxin | 6 | -2614.611 | -2.045 | 0.087 | -1.049 |
| 2-bromo-1-chlorodibenzo*-p-*dioxin | 6 | -2614.530 | -2.337 | 0.099 | -0.812 |
| 2-bromo-3-chlorodibenzo*-p-*dioxin | 6 | -2614.602 | -1.446 | 0.087 | -2.208 |
| 2-bromo-4-chlorodibenzo*-p-*dioxin | 6 | -2614.680 | -0.635 | 0.061 | -3.086 |
| 2-bromo-6-chlorodibenzo*-p-*dioxin | 6 | -2614.701 | -0.251 | 0.018 | -2.707 |
| 2-bromo-7-chlorodibenzo*-p-*dioxin | 6 | -2614.787 | 0.030 | 0.000 | -2.766 |
| 2-bromo-8-chlorodibenzo*-p-*dioxin | 6 | -2614.787 | -1.303 | 0.050 | -1.489 |
| 2-bromo-9-chlorodibenzo*-p-*dioxin | 6 | -2614.699 | -2.363 | 0.121 | -1.301 |
| 1,2-dibromodibenzo*-p-*dioxin | 6 | -2588.054 | -2.321 | 0.099 | -5.821 |
| 1,3-dibromodibenzo*-p-*dioxin | 6 | -2588.119 | -1.339 | 0.092 | -7.525 |
| 1,4-dibromodibenzo*-p-*dioxin | 6 | -2588.046 | -0.439 | 0.037 | -7.849 |
| 1,7-dibromodibenzo*-p-*dioxin | 6 | -2588.142 | 0.282 | -0.039 | -7.251 |
| 1,8-dibromodibenzo*-p-*dioxin | 6 | -2588.140 | -1.004 | 0.023 | -6.376 |
| 1,9-dibromodibenzo*-p-*dioxin | 6 | -2588.052 | -1.964 | 0.093 | -6.356 |
| 2,3-dibromodibenzo*-p-*dioxin | 6 | -2588.127 | -1.469 | 0.088 | -7.168 |
| 2,8-dibromodibenzo*-p-*dioxin | 6 | -2588.220 | -1.286 | 0.049 | -6.491 |
| 1,2,3-trichlorodibenzo*-p-*dioxin | 5 | -2881.994 | -2.223 | 0.119 | 2.697 |
| 1,2,4-trichlorodibenzo*-p-*dioxin | 5 | -2882.044 | -1.468 | 0.082 | 2.208 |
| 1,2,6-trichlorodibenzo*-p-*dioxin | 5 | -2882.074 | -1.075 | 0.065 | 1.896 |
| 1,2,7-trichlorodibenzo*-p-*dioxin | 5 | -2882.159 | -0.791 | 0.031 | 2.246 |
| 1,2,8-trichlorodibenzo*-p-*dioxin | 5 | -2882.157 | -2.099 | 0.076 | 3.604 |
| 1,2,9-trichlorodibenzo*-p-*dioxin | 5 | -2882.064 | -3.105 | 0.150 | 3.609 |
| 1,3,6-trichlorodibenzo*-p-*dioxin | 5 | -2882.205 | -0.110 | 0.041 | 0.679 |
| 1,3,7-trichlorodibenzo*-p-*dioxin | 5 | -2882.288 | 0.177 | -0.001 | 1.231 |
| 1,3,8-trichlorodibenzo*-p-*dioxin | 5 | -2882.289 | -1.124 | 0.050 | 2.421 |
| 1,3,9-trichlorodibenzo*-p-*dioxin | 5 | -2882.195 | -2.124 | 0.119 | 2.543 |
| 1,4,7-trichlorodibenzo*-p-*dioxin | 5 | -2882.205 | 1.117 | -0.059 | 0.905 |
| 1,7,8-trichlorodibenzo*-p-*dioxin | 5 | -2882.146 | 0.214 | -0.047 | 2.327 |
| 2,3,7-trichlorodibenzo*-p-*dioxin | 5 | -2882.232 | 0.075 | 0.012 | 1.080 |
| 1-bromo-2,3-dichlorodibenzo*-p-*dioxin | 5 | -2855.401 | -2.149 | 0.116 | -2.369 |
| 1-bromo-2,4-dichlorodibenzo*-p-*dioxin | 5 | -2855.457 | -1.412 | 0.083 | -2.925 |
| 1-bromo-2,6-dichlorodibenzo*-p-*dioxin | 5 | -2855.486 | -1.006 | 0.061 | -3.133 |
| 1-bromo-2,7-dichlorodibenzo*-p-*dioxin | 5 | -2855.572 | -0.726 | 0.028 | -2.801 |
| 1-bromo-2,8-dichlorodibenzo*-p-*dioxin | 5 | -2855.568 | -2.038 | 0.067 | -1.279 |
| 1-bromo-2,9-dichlorodibenzo*-p-*dioxin | 5 | -2855.476 | -3.041 | 0.135 | -1.125 |
| 1-bromo-3,4-dichlorodibenzo*-p-*dioxin | 5 | -2855.483 | -0.612 | 0.082 | -4.440 |
| 1-bromo-3,6-dichlorodibenzo*-p-*dioxin | 5 | -2855.640 | -0.053 | 0.040 | -4.400 |
| 1-bromo-3,7-dichlorodibenzo*-p-*dioxin | 5 | -2855.724 | 0.230 | 0.005 | -4.022 |
| 1-bromo-3,8-dichlorodibenzo*-p-*dioxin | 5 | -2855.725 | -1.072 | 0.049 | -2.649 |
| 1-bromo-3,9-dichlorodibenzo*-p-*dioxin | 5 | -2855.631 | -2.071 | 0.108 | -2.269 |
| 1-bromo-4,6-dichlorodibenzo*-p-*dioxin | 5 | -2855.555 | 0.837 | -0.001 | -5.071 |
| 1-bromo-4,7-dichlorodibenzo*-p-*dioxin | 5 | -2855.648 | 1.156 | -0.057 | -4.216 |
| 1-bromo-4,9-dichlorodibenzo*-p-*dioxin | 5 | -2855.555 | -1.133 | 0.044 | -2.433 |
| 1-bromo-6,7-dichlorodibenzo*-p-*dioxin | 5 | -2855.515 | 1.114 | -0.073 | -3.744 |
| 1-bromo-6,8-dichlorodibenzo*-p-*dioxin | 5 | -2855.645 | 0.152 | -0.015 | -3.367 |
| 1-bromo-6,9-dichlorodibenzo*-p-*dioxin | 5 | -2855.553 | -0.747 | 0.051 | -3.361 |
| 1-bromo-7,8-dichlorodibenzo*-p-*dioxin | 5 | -2855.587 | 0.245 | -0.053 | -2.571 |
| 1-bromo-7,9-dichlorodibenzo*-p-*dioxin | 5 | -2855.636 | -0.474 | 0.005 | -2.679 |
| 1-bromo-8,9-dichlorodibenzo*-p-*dioxin | 5 | -2855.504 | -1.637 | 0.066 | -2.040 |
| 2-bromo-1,3-dichlorodibenzo*-p-*dioxin | 5 | -2855.370 | -2.170 | 0.112 | -2.230 |
| 2-bromo-1,4-dichlorodibenzo*-p-*dioxin | 5 | -2855.452 | -1.416 | 0.076 | -2.737 |
| 2-bromo-1,6-dichlorodibenzo*-p-*dioxin | 5 | -2855.487 | -1.031 | 0.060 | -3.059 |
| 2-bromo-1,7-dichlorodibenzo*-p-*dioxin | 5 | -2855.570 | -0.743 | 0.030 | -2.820 |
| 2-bromo-1,8-dichlorodibenzo*-p-*dioxin | 5 | -2855.569 | -2.051 | 0.068 | -1.280 |
| 2-bromo-1,9-dichlorodibenzo*-p-*dioxin | 5 | -2855.476 | -3.054 | 0.138 | -1.177 |
| 2-bromo-3,4-dichlorodibenzo*-p-*dioxin | 5 | -2855.398 | -0.718 | 0.079 | -4.173 |
| 2-bromo-3,6-dichlorodibenzo*-p-*dioxin | 5 | -2855.555 | -0.180 | 0.029 | -3.885 |
| 2-bromo-3,7-dichlorodibenzo*-p-*dioxin | 5 | -2855.639 | 0.107 | 0.015 | -4.060 |
| 2-bromo-3,8-dichlorodibenzo*-p-*dioxin | 5 | -2855.640 | -1.202 | 0.058 | -2.647 |
| 2-bromo-3,9-dichlorodibenzo*-p-*dioxin | 5 | -2855.554 | -2.238 | 0.115 | -2.142 |
| 2-bromo-4,6-dichlorodibenzo*-p-*dioxin | 5 | -2855.625 | 0.555 | 0.013 | -4.876 |
| 2-bromo-4,7-dichlorodibenzo*-p-*dioxin | 5 | -2855.718 | 0.883 | -0.013 | -4.818 |
| 2-bromo-4,8-dichlorodibenzo*-p-*dioxin | 5 | -2855.718 | -0.414 | 0.015 | -3.039 |
| 2-bromo-4,9-dichlorodibenzo*-p-*dioxin | 5 | -2855.634 | -1.448 | 0.068 | -2.433 |
| 2-bromo-6,7-dichlorodibenzo*-p-*dioxin | 5 | -2855.592 | 0.821 | -0.046 | -3.865 |
| 2-bromo-6,8-dichlorodibenzo*-p-*dioxin | 5 | -2855.722 | -0.143 | 0.008 | -3.380 |
| 2-bromo-6,9-dichlorodibenzo*-p-*dioxin | 5 | -2855.638 | -1.080 | 0.068 | -3.143 |
| 2-bromo-7,8-dichlorodibenzo*-p-*dioxin | 5 | -2855.664 | -0.040 | -0.009 | -3.148 |
| 2-bromo-7,9-dichlorodibenzo*-p-*dioxin | 5 | -2855.721 | -0.799 | 0.044 | -3.047 |
| 2-bromo-8,9-dichlorodibenzo*-p-*dioxin | 5 | -2855.590 | -1.956 | 0.097 | -2.213 |
| 1,2-dibromo-3-chlorodibenzo*-p-*dioxin | 5 | -2828.891 | -2.151 | 0.107 | -7.116 |
| 1,2-dibromo-4-chlorodibenzo*-p-*dioxin | 5 | -2828.979 | -1.400 | 0.076 | -7.746 |
| 1,2-dibromo-6-chlorodibenzo*-p-*dioxin | 5 | -2829.011 | -1.005 | 0.057 | -8.009 |
| 1,2-dibromo-7-chlorodibenzo*-p-*dioxin | 5 | -2829.095 | -0.722 | 0.028 | -7.787 |
| 1,2-dibromo-8-chlorodibenzo*-p-*dioxin | 5 | -2829.093 | -2.029 | 0.063 | -6.171 |
| 1,2-dibromo-9-chlorodibenzo*-p-*dioxin | 5 | -2828.999 | -3.030 | 0.131 | -6.021 |
| 1,3-dibromo-2-chlorodibenzo*-p-*dioxin | 5 | -2828.795 | -2.163 | 0.127 | -7.630 |
| 1,3-dibromo-4-chlorodibenzo*-p-*dioxin | 5 | -2828.894 | -0.615 | 0.076 | -9.278 |
| 1,3-dibromo-6-chlorodibenzo*-p-*dioxin | 5 | -2829.072 | -0.067 | 0.037 | -9.291 |
| 1,3-dibromo-7-chlorodibenzo*-p-*dioxin | 5 | -2829.157 | 0.219 | 0.005 | -8.997 |
| 1,3-dibromo-8-chlorodibenzo*-p-*dioxin | 5 | -2829.157 | -1.078 | 0.047 | -7.581 |
| 1,3-dibromo-9-chlorodibenzo*-p-*dioxin | 5 | -2829.064 | -2.076 | 0.109 | -7.280 |
| 1,4-dibromo-2-chlorodibenzo*-p-*dioxin | 5 | -2828.892 | -1.499 | 0.083 | -7.752 |
| 1,4-dibromo-6-chlorodibenzo*-p-*dioxin | 5 | -2828.994 | 0.755 | 0.007 | -10.115 |
| 1,4-dibromo-7-chlorodibenzo*-p-*dioxin | 5 | -2829.087 | 1.085 | -0.052 | -9.203 |
| 1,6-dibromo-2-chlorodibenzo*-p-*dioxin | 5 | -2828.928 | -1.044 | 0.079 | -8.521 |
| 1,6-dibromo-3-chlorodibenzo*-p-*dioxin | 5 | -2829.081 | -0.093 | 0.035 | -9.187 |
| 1,6-dibromo-4-chlorodibenzo*-p-*dioxin | 5 | -2828.996 | 0.793 | -0.011 | -9.720 |
| 1,7-dibromo-2-chlorodibenzo*-p-*dioxin | 5 | -2829.004 | -0.756 | 0.031 | -7.817 |
| 1,7-dibromo-3-chlorodibenzo*-p-*dioxin | 5 | -2829.158 | 0.197 | -0.001 | -8.798 |
| 1,7-dibromo-4-chlorodibenzo*-p-*dioxin | 5 | -2829.081 | 1.121 | -0.058 | -9.118 |
| 1,7-dibromo-6-chlorodibenzo*-p-*dioxin | 5 | -2828.927 | 1.071 | -0.071 | -8.713 |
| 1,7-dibromo-8-chlorodibenzo*-p-*dioxin | 5 | -2828.995 | 0.214 | -0.055 | -7.459 |
| 1,7-dibromo-9-chlorodibenzo*-p-*dioxin | 5 | -2829.066 | -0.516 | 0.005 | -7.594 |
| 1,8-dibromo-2-chlorodibenzo*-p-*dioxin | 5 | -2829.002 | -2.017 | 0.069 | -6.367 |
| 1,8-dibromo-3-chlorodibenzo*-p-*dioxin | 5 | -2829.157 | -1.057 | 0.047 | -7.622 |
| 1,8-dibromo-4-chlorodibenzo*-p-*dioxin | 5 | -2829.081 | -0.124 | -0.009 | -7.985 |
| 1,8-dibromo-6-chlorodibenzo*-p-*dioxin | 5 | -2829.074 | 0.171 | -0.019 | -8.296 |
| 1,8-dibromo-7-chlorodibenzo*-p-*dioxin | 5 | -2828.994 | 0.280 | -0.038 | -8.028 |
| 1,8-dibromo-9-chlorodibenzo*-p-*dioxin | 5 | -2828.916 | -1.619 | 0.061 | -6.945 |
| 1,9-dibromo-2-chlorodibenzo*-p-*dioxin | 5 | -2828.917 | -2.964 | 0.140 | -6.397 |
| 1,9-dibromo-3-chlorodibenzo*-p-*dioxin | 5 | -2829.072 | -1.995 | 0.106 | -7.357 |
| 1,9-dibromo-4-chlorodibenzo*-p-*dioxin | 5 | -2828.996 | -1.056 | 0.047 | -7.654 |
| 2,3-dibromo-1-chlorodibenzo*-p-*dioxin | 5 | -2828.893 | -2.194 | 0.112 | -7.163 |
| 2,3-dibromo-6-chlorodibenzo*-p-*dioxin | 5 | -2829.079 | -0.209 | 0.033 | -8.911 |
| 2,3-dibromo-7-chlorodibenzo*-p-*dioxin | 5 | -2829.164 | 0.083 | 0.014 | -8.966 |
| 2,7-dibromo-1-chlorodibenzo*-p-*dioxin | 5 | -2829.004 | -0.775 | 0.032 | -7.806 |
| 2,7-dibromo-3-chlorodibenzo*-p-*dioxin | 5 | -2829.072 | 0.072 | 0.014 | -8.962 |
| 2,7-dibromo-4-chlorodibenzo*-p-*dioxin | 5 | -2829.150 | 0.846 | -0.014 | -9.716 |
| 2,8-dibromo-1-chlorodibenzo*-p-*dioxin | 5 | -2829.002 | -2.031 | 0.069 | -6.340 |
| 2,8-dibromo-3-chlorodibenzo*-p-*dioxin | 5 | -2829.073 | -1.188 | 0.057 | -7.644 |
| 2,8-dibromo-4-chlorodibenzo*-p-*dioxin | 5 | -2829.151 | -0.402 | 0.015 | -8.057 |
| 1,2,3-tribromodibenzo*-p-*dioxin | 5 | -2802.416 | -2.165 | 0.110 | -12.145 |
| 1,2,4-tribromodibenzo*-p-*dioxin | 5 | -2802.416 | -1.488 | 0.079 | -12.648 |
| 1,2,6-tribromodibenzo*-p-*dioxin | 5 | -2802.452 | -1.046 | 0.065 | -13.132 |
| 1,2,7-tribromodibenzo*-p-*dioxin | 5 | -2802.528 | -0.752 | 0.030 | -12.777 |
| 1,2,8-tribromodibenzo*-p-*dioxin | 5 | -2802.526 | -2.009 | 0.065 | -11.257 |
| 1,2,9-tribromodibenzo*-p-*dioxin | 5 | -2802.440 | -2.952 | 0.135 | -11.269 |
| 1,3,6-tribromodibenzo*-p-*dioxin | 5 | -2802.513 | -0.108 | 0.033 | -14.102 |
| 1,3,7-tribromodibenzo*-p-*dioxin | 5 | -2802.590 | 0.186 | 0.004 | -13.902 |
| 1,3,8-tribromodibenzo*-p-*dioxin | 5 | -2802.589 | -1.063 | 0.046 | -12.580 |
| 1,3,9-tribromodibenzo*-p-*dioxin | 5 | -2802.505 | -2.001 | 0.106 | -12.341 |
| 1,4,6-tribromodibenzo*-p-*dioxin | 5 | -2802.435 | 0.722 | -0.002 | -14.811 |
| 1,4,7-tribromodibenzo*-p-*dioxin | 5 | -2802.520 | 1.049 | -0.053 | -14.103 |
| 1,7,8-tribromodibenzo*-p-*dioxin | 5 | -2802.519 | 0.244 | -0.048 | -12.678 |
| 2,3,7-tribromodibenzo*-p-*dioxin | 5 | -2802.597 | 0.047 | 0.016 | -13.944 |
| 1,2,3,4-tetrachlorodibenzo*-p-*dioxin | 4 | -3122.784 | -1.497 | 0.103 | 0.942 |
| 1,2,3,6-tetrachlorodibenzo*-p-*dioxin | 4 | -3122.946 | -0.953 | 0.073 | 0.700 |
| 1,2,3,7-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.029 | -0.659 | 0.047 | 0.823 |
| 1,2,3,8-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.028 | -1.946 | 0.084 | 2.349 |
| 1,2,3,9-tetrachlorodibenzo*-p-*dioxin | 4 | -3122.937 | -2.932 | 0.145 | 2.653 |
| 1,2,4,6-tetrachlorodibenzo*-p-*dioxin | 4 | -3122.988 | -0.275 | 0.047 | 0.074 |
| 1,2,4,7-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.080 | 0.055 | 0.010 | 0.414 |
| 1,2,4,8-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.078 | -1.217 | 0.035 | 2.222 |
| 1,2,4,9-tetrachlorodibenzo*-p-*dioxin | 4 | -3122.988 | -2.198 | 0.094 | 2.569 |
| 1,2,6,7-tetrachlorodibenzo*-p-*dioxin | 4 | -3122.962 | 0.000 | 0.001 | 0.732 |
| 1,2,6,8-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.090 | -0.940 | 0.044 | 1.456 |
| 1,2,6,9-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.001 | -1.822 | 0.105 | 1.559 |
| 1,2,7,8-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.032 | -0.836 | 0.020 | 1.867 |
| 1,2,7,9-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.083 | -1.538 | 0.077 | 1.753 |
| 1,2,8,9-tetrachlorodibenzo*-p-*dioxin | 4 | -3122.952 | -2.682 | 0.122 | 2.770 |
| 1,3,6,8-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.222 | 0.000 | 0.002 | 0.755 |
| 1,3,6,9-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.131 | -0.880 | 0.060 | 0.932 |
| 1,3,7,8-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.162 | 0.114 | -0.018 | 1.043 |
| 1,3,7,9-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.211 | -0.589 | 0.032 | 1.112 |
| 1,4,7,8-tetrachlorodibenzo*-p-*dioxin | 4 | -3123.079 | 1.033 | -0.084 | 0.965 |
| 1-bromo-2,3,4-trichlorodibenzo*-p-*dioxin | 4 | -3096.192 | -1.432 | 0.103 | -4.184 |
| 1-bromo-2,3,6-trichlorodibenzo*-p-*dioxin | 4 | -3096.352 | -0.868 | 0.071 | -4.412 |
| 1-bromo-2,3,7-trichlorodibenzo*-p-*dioxin | 4 | -3096.436 | -0.577 | 0.043 | -4.232 |
| 1-bromo-2,3,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.435 | -1.866 | 0.076 | -2.598 |
| 1-bromo-2,3,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.343 | -2.852 | 0.136 | -2.269 |
| 1-bromo-2,4,6-trichlorodibenzo*-p-*dioxin | 4 | -3096.401 | -0.209 | 0.048 | -5.079 |
| 1-bromo-2,4,7-trichlorodibenzo*-p-*dioxin | 4 | -3096.494 | 0.118 | 0.009 | -4.681 |
| 1-bromo-2,4,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.491 | -1.158 | 0.033 | -2.839 |
| 1-bromo-2,4,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.402 | -2.137 | 0.088 | -2.393 |
| 1-bromo-2,6,7-trichlorodibenzo*-p-*dioxin | 4 | -3096.374 | 0.073 | -0.002 | -4.331 |
| 1-bromo-2,6,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.502 | -0.868 | 0.040 | -3.579 |
| 1-bromo-2,6,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.413 | -1.747 | 0.094 | -3.300 |
| 1-bromo-2,7,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.445 | -0.771 | 0.014 | -3.102 |
| 1-bromo-2,7,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.496 | -1.469 | 0.065 | -3.068 |
| 1-bromo-2,8,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.363 | -2.617 | 0.107 | -1.966 |
| 1-bromo-3,4,6-trichlorodibenzo*-p-*dioxin | 4 | -3096.427 | 0.569 | 0.029 | -6.084 |
| 1-bromo-3,4,7-trichlorodibenzo*-p-*dioxin | 4 | -3096.517 | 0.894 | -0.004 | -5.838 |
| 1-bromo-3,4,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.518 | -0.377 | 0.026 | -4.161 |
| 1-bromo-3,4,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.426 | -1.360 | 0.072 | -3.474 |
| 1-bromo-3,6,7-trichlorodibenzo*-p-*dioxin | 4 | -3096.526 | 1.001 | -0.039 | -5.135 |
| 1-bromo-3,6,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.657 | 0.062 | -0.002 | -4.256 |
| 1-bromo-3,6,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.566 | -0.815 | 0.056 | -4.085 |
| 1-bromo-3,7,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.598 | 0.170 | -0.020 | -4.009 |
| 1-bromo-3,7,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.647 | -0.531 | 0.026 | -3.840 |
| 1-bromo-3,8,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.518 | -1.666 | 0.081 | -3.099 |
| 1-bromo-4,6,7-trichlorodibenzo*-p-*dioxin | 4 | -3096.444 | 1.870 | -0.088 | -5.557 |
| 1-bromo-4,6,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.573 | 0.927 | -0.054 | -4.593 |
| 1-bromo-4,6,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.483 | 0.049 | 0.003 | -4.394 |
| 1-bromo-4,7,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.522 | 1.074 | -0.084 | -4.108 |
| 1-bromo-4,7,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.574 | 0.371 | -0.038 | -3.934 |
| 1-bromo-4,8,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.443 | -0.750 | 0.016 | -3.195 |
| 1-bromo-6,7,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.386 | 0.994 | -0.078 | -4.135 |
| 1-bromo-6,7,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.428 | 0.321 | -0.032 | -4.021 |
| 1-bromo-6,8,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.428 | -0.468 | 0.021 | -3.873 |
| 1-bromo-7,8,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.377 | -0.374 | 0.002 | -3.571 |
| 2-bromo-1,3,4-trichlorodibenzo*-p-*dioxin | 4 | -3096.154 | -1.443 | 0.092 | -3.884 |
| 2-bromo-1,3,6-trichlorodibenzo*-p-*dioxin | 4 | -3096.321 | -0.901 | 0.066 | -4.225 |
| 2-bromo-1,3,7-trichlorodibenzo*-p-*dioxin | 4 | -3096.403 | -0.606 | 0.044 | -4.208 |
| 2-bromo-1,3,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.404 | -1.891 | 0.076 | -2.556 |
| 2-bromo-1,3,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.311 | -2.872 | 0.132 | -2.132 |
| 2-bromo-1,4,6-trichlorodibenzo*-p-*dioxin | 4 | -3096.396 | -0.223 | 0.039 | -4.820 |
| 2-bromo-1,4,7-trichlorodibenzo*-p-*dioxin | 4 | -3096.486 | 0.111 | 0.008 | -4.643 |
| 2-bromo-1,4,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.486 | -1.160 | 0.029 | -2.733 |
| 2-bromo-1,4,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.395 | -2.138 | 0.085 | -2.314 |
| 2-bromo-1,6,7-trichlorodibenzo*-p-*dioxin | 4 | -3096.373 | 0.047 | -0.003 | -4.255 |
| 2-bromo-1,6,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.503 | -0.890 | 0.046 | -3.692 |
| 2-bromo-1,6,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.412 | -1.770 | 0.099 | -3.385 |
| 2-bromo-1,7,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.444 | -0.784 | 0.019 | -3.207 |
| 2-bromo-1,7,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.494 | -1.484 | 0.073 | -3.248 |
| 2-bromo-3,4,6-trichlorodibenzo*-p-*dioxin | 4 | -3096.341 | 0.452 | 0.027 | -5.822 |
| 2-bromo-3,4,7-trichlorodibenzo*-p-*dioxin | 4 | -3096.431 | 0.781 | 0.010 | -6.000 |
| 2-bromo-3,4,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.432 | -0.499 | 0.033 | -4.124 |
| 2-bromo-3,4,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.348 | -1.517 | 0.083 | -3.471 |
| 2-bromo-3,6,7-trichlorodibenzo*-p-*dioxin | 4 | -3096.440 | 0.868 | -0.036 | -4.972 |
| 2-bromo-3,6,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.571 | -0.080 | 0.012 | -4.362 |
| 2-bromo-3,6,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.487 | -0.994 | 0.060 | -3.858 |
| 2-bromo-3,7,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.512 | 0.035 | -0.002 | -4.231 |
| 2-bromo-3,7,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.568 | -0.705 | 0.041 | -3.908 |
| 2-bromo-3,8,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.440 | -1.841 | 0.090 | -3.009 |
| 2-bromo-4,6,7-trichlorodibenzo*-p-*dioxin | 4 | -3096.512 | 1.585 | -0.055 | -5.850 |
| 2-bromo-4,6,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.641 | 0.638 | -0.024 | -4.801 |
| 2-bromo-4,6,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.559 | -0.277 | 0.027 | -4.373 |
| 2-bromo-4,7,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.591 | 0.793 | -0.040 | -4.694 |
| 2-bromo-4,7,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.649 | 0.052 | -0.003 | -4.213 |
| 2-bromo-4,8,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.519 | -1.067 | 0.036 | -3.088 |
| 2-bromo-6,7,8-trichlorodibenzo*-p-*dioxin | 4 | -3096.462 | 0.694 | -0.044 | -4.424 |
| 2-bromo-6,7,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.511 | -0.017 | 0.003 | -4.261 |
| 2-bromo-6,8,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.511 | -0.804 | 0.051 | -3.987 |
| 2-bromo-7,8,9-trichlorodibenzo*-p-*dioxin | 4 | -3096.460 | -0.701 | 0.039 | -3.884 |
| 1,2-dibromo-3,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.678 | -1.429 | 0.093 | -8.915 |
| 1,2-dibromo-3,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.842 | -0.871 | 0.066 | -9.262 |
| 1,2-dibromo-3,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.925 | -0.580 | 0.043 | -9.211 |
| 1,2-dibromo-3,8-dichlorodibenzo*-p-*dioxin | 4 | -3069.925 | -1.863 | 0.072 | -7.485 |
| 1,2-dibromo-3,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.832 | -2.845 | 0.127 | -7.033 |
| 1,2-dibromo-4,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.922 | -0.197 | 0.039 | -9.848 |
| 1,2-dibromo-4,7-dichlorodibenzo*-p-*dioxin | 4 | -3070.013 | 0.133 | 0.012 | -9.767 |
| 1,2-dibromo-4,8-dichlorodibenzo*-p-*dioxin | 4 | -3070.012 | -1.137 | 0.029 | -7.755 |
| 1,2-dibromo-4,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.921 | -2.115 | 0.080 | -7.207 |
| 1,2-dibromo-6,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.898 | 0.077 | -0.002 | -9.317 |
| 1,2-dibromo-6,8-dichlorodibenzo*-p-*dioxin | 4 | -3070.026 | -0.860 | 0.038 | -8.521 |
| 1,2-dibromo-6,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.936 | -1.737 | 0.093 | -8.272 |
| 1,2-dibromo-7,8-dichlorodibenzo*-p-*dioxin | 4 | -3069.968 | -0.760 | 0.014 | -8.102 |
| 1,2-dibromo-7,9-dichlorodibenzo*-p-*dioxin | 4 | -3070.018 | -1.457 | 0.067 | -8.122 |
| 1,2-dibromo-8,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.887 | -2.602 | 0.102 | -6.844 |
| 1,3-dibromo-2,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.552 | -1.439 | 0.107 | -9.283 |
| 1,3-dibromo-2,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.745 | -0.888 | 0.085 | -9.740 |
| 1,3-dibromo-2,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.830 | -0.596 | 0.049 | -9.354 |
| 1,3-dibromo-2,8-dichlorodibenzo*-p-*dioxin | 4 | -3069.828 | -1.877 | 0.076 | -7.580 |
| 1,3-dibromo-2,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.738 | -2.862 | 0.135 | -7.226 |
| 1,3-dibromo-4,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.837 | 0.558 | 0.024 | -10.933 |
| 1,3-dibromo-4,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.928 | 0.887 | -0.010 | -10.669 |
| 1,3-dibromo-4,8-dichlorodibenzo*-p-*dioxin | 4 | -3069.927 | -0.381 | 0.023 | -9.076 |
| 1,3-dibromo-4,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.837 | -1.361 | 0.076 | -8.576 |
| 1,3-dibromo-6,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.958 | 0.986 | -0.033 | -10.257 |
| 1,3-dibromo-6,8-dichlorodibenzo*-p-*dioxin | 4 | -3070.087 | 0.053 | 0.008 | -9.495 |
| 1,3-dibromo-6,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.998 | -0.825 | 0.069 | -9.399 |
| 1,3-dibromo-7,8-dichlorodibenzo*-p-*dioxin | 4 | -3070.030 | 0.160 | -0.020 | -8.985 |
| 1,3-dibromo-7,9-dichlorodibenzo*-p-*dioxin | 4 | -3070.080 | -0.540 | 0.026 | -8.818 |
| 1,3-dibromo-8,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.950 | -1.670 | 0.079 | -8.035 |
| 1,4-dibromo-2,3-dichlorodibenzo*-p-*dioxin | 4 | -3069.596 | -1.518 | 0.102 | -8.993 |
| 1,4-dibromo-2,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.836 | -0.303 | 0.061 | -10.231 |
| 1,4-dibromo-2,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.928 | 0.033 | 0.016 | -9.694 |
| 1,4-dibromo-2,8-dichlorodibenzo*-p-*dioxin | 4 | -3069.926 | -1.243 | 0.032 | -7.644 |
| 1,4-dibromo-2,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.836 | -2.222 | 0.087 | -7.198 |
| 1,4-dibromo-6,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.882 | 1.793 | -0.082 | -10.558 |
| 1,4-dibromo-6,8-dichlorodibenzo*-p-*dioxin | 4 | -3070.012 | 0.849 | -0.052 | -9.489 |
| 1,4-dibromo-6,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.922 | -0.030 | 0.007 | -9.340 |
| 1,4-dibromo-7,8-dichlorodibenzo*-p-*dioxin | 4 | -3069.961 | 1.006 | -0.084 | -8.971 |
| 1,6-dibromo-2,3-dichlorodibenzo*-p-*dioxin | 4 | -3069.793 | -0.908 | 0.084 | -9.667 |
| 1,6-dibromo-2,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.843 | -0.254 | 0.055 | -10.168 |
| 1,6-dibromo-2,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.788 | 0.000 | 0.006 | -9.397 |
| 1,6-dibromo-2,8-dichlorodibenzo*-p-*dioxin | 4 | -3069.939 | -0.928 | 0.055 | -8.848 |
| 1,6-dibromo-2,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.857 | -1.793 | 0.109 | -8.594 |
| 1,6-dibromo-3,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.867 | 0.524 | 0.020 | -10.758 |
| 1,6-dibromo-3,8-dichlorodibenzo*-p-*dioxin | 4 | -3070.092 | 0.000 | 0.006 | -9.340 |
| 1,6-dibromo-3,9-dichlorodibenzo*-p-*dioxin | 4 | -3070.009 | -0.861 | 0.071 | -9.380 |
| 1,6-dibromo-4,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.927 | 0.001 | 0.014 | -9.580 |
| 1,7-dibromo-2,3-dichlorodibenzo*-p-*dioxin | 4 | -3069.868 | -0.612 | 0.045 | -9.212 |
| 1,7-dibromo-2,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.925 | 0.081 | 0.011 | -9.657 |
| 1,7-dibromo-2,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.786 | 0.026 | 0.001 | -9.318 |
| 1,7-dibromo-2,8-dichlorodibenzo*-p-*dioxin | 4 | -3069.852 | -0.800 | 0.018 | -8.151 |
| 1,7-dibromo-2,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.924 | -1.513 | 0.071 | -8.136 |
| 1,7-dibromo-3,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.950 | 0.857 | -0.002 | -10.814 |
| 1,7-dibromo-3,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.939 | 0.953 | -0.038 | -10.067 |
| 1,7-dibromo-3,8-dichlorodibenzo*-p-*dioxin | 4 | -3070.006 | 0.137 | -0.020 | -8.945 |
| 1,7-dibromo-3,9-dichlorodibenzo*-p-*dioxin | 4 | -3070.077 | -0.578 | 0.030 | -8.849 |
| 1,7-dibromo-4,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.855 | 1.819 | -0.088 | -10.458 |
| 1,7-dibromo-4,8-dichlorodibenzo*-p-*dioxin | 4 | -3069.929 | 1.037 | -0.085 | -9.011 |
| 1,7-dibromo-4,9-dichlorodibenzo*-p-*dioxin | 4 | -3070.002 | 0.322 | -0.038 | -8.836 |
| 1,7-dibromo-6,8-dichlorodibenzo*-p-*dioxin | 4 | -3069.761 | 0.944 | -0.081 | -8.967 |
| 1,7-dibromo-6,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.836 | 0.271 | -0.031 | -8.951 |
| 1,7-dibromo-8,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.780 | -0.411 | -0.004 | -8.344 |
| 1,8-dibromo-2,3-dichlorodibenzo*-p-*dioxin | 4 | -3069.867 | -1.849 | 0.078 | -7.679 |
| 1,8-dibromo-2,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.924 | -1.142 | 0.043 | -8.125 |
| 1,8-dibromo-2,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.931 | -0.847 | 0.047 | -8.798 |
| 1,8-dibromo-2,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.852 | -0.735 | 0.018 | -8.276 |
| 1,8-dibromo-2,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.776 | -2.598 | 0.116 | -7.236 |
| 1,8-dibromo-3,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.950 | -0.366 | 0.022 | -9.075 |
| 1,8-dibromo-3,6-dichlorodibenzo*-p-*dioxin | 4 | -3070.085 | 0.078 | 0.004 | -9.440 |
| 1,8-dibromo-3,7-dichlorodibenzo*-p-*dioxin | 4 | -3070.004 | 0.198 | -0.016 | -9.167 |
| 1,8-dibromo-3,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.929 | -1.651 | 0.077 | -8.024 |
| 1,8-dibromo-4,6-dichlorodibenzo*-p-*dioxin | 4 | -3070.002 | 0.942 | -0.046 | -9.826 |
| 1,8-dibromo-4,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.930 | 1.101 | -0.071 | -9.498 |
| 1,8-dibromo-4,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.855 | -0.737 | 0.012 | -8.116 |
| 1,8-dibromo-6,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.789 | 1.019 | -0.070 | -9.392 |
| 1,8-dibromo-6,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.835 | -0.450 | 0.017 | -8.804 |
| 1,8-dibromo-7,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.752 | -0.345 | 0.000 | -8.581 |
| 1,9-dibromo-2,3-dichlorodibenzo*-p-*dioxin | 4 | -3069.785 | -2.780 | 0.135 | -7.376 |
| 1,9-dibromo-2,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.842 | -2.062 | 0.091 | -7.610 |
| 1,9-dibromo-2,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.856 | -1.684 | 0.098 | -8.519 |
| 1,9-dibromo-2,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.932 | -1.378 | 0.069 | -8.343 |
| 1,9-dibromo-2,8-dichlorodibenzo*-p-*dioxin | 4 | -3069.776 | -2.526 | 0.116 | -7.375 |
| 1,9-dibromo-3,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.868 | -1.284 | 0.074 | -8.667 |
| 1,9-dibromo-3,6-dichlorodibenzo*-p-*dioxin | 4 | -3070.010 | -0.752 | 0.050 | -9.045 |
| 1,9-dibromo-3,7-dichlorodibenzo*-p-*dioxin | 4 | -3070.084 | -0.440 | 0.022 | -8.906 |
| 1,9-dibromo-4,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.927 | 0.114 | -0.001 | -9.409 |
| 2,3-dibromo-1,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.644 | -1.464 | 0.091 | -8.802 |
| 2,3-dibromo-1,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.843 | -0.930 | 0.067 | -9.174 |
| 2,3-dibromo-1,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.926 | -0.632 | 0.042 | -9.085 |
| 2,3-dibromo-1,8-dichlorodibenzo*-p-*dioxin | 4 | -3069.926 | -1.911 | 0.077 | -7.522 |
| 2,3-dibromo-1,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.834 | -2.893 | 0.136 | -7.174 |
| 2,3-dibromo-6,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.964 | 0.839 | -0.030 | -10.050 |
| 2,3-dibromo-6,8-dichlorodibenzo*-p-*dioxin | 4 | -3070.093 | -0.103 | 0.011 | -9.270 |
| 2,3-dibromo-6,9-dichlorodibenzo*-p-*dioxin | 4 | -3070.011 | -1.017 | 0.064 | -8.896 |
| 2,3-dibromo-7,8-dichlorodibenzo*-p-*dioxin | 4 | -3070.036 | 0.013 | -0.001 | -9.193 |
| 2,7-dibromo-1,3-dichlorodibenzo*-p-*dioxin | 4 | -3069.836 | -0.641 | 0.047 | -9.214 |
| 2,7-dibromo-1,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.918 | 0.073 | 0.008 | -9.565 |
| 2,7-dibromo-1,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.786 | 0.000 | 0.001 | -9.267 |
| 2,7-dibromo-1,8-dichlorodibenzo*-p-*dioxin | 4 | -3069.852 | -0.816 | 0.022 | -8.224 |
| 2,7-dibromo-1,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.923 | -1.530 | 0.080 | -8.337 |
| 2,7-dibromo-3,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.863 | 0.742 | 0.010 | -10.920 |
| 2,7-dibromo-3,8-dichlorodibenzo*-p-*dioxin | 4 | -3069.920 | 0.000 | 0.001 | -9.242 |
| 2,7-dibromo-3,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.998 | -0.755 | 0.048 | -8.989 |
| 2,7-dibromo-4,9-dichlorodibenzo*-p-*dioxin | 4 | -3070.078 | 0.000 | 0.000 | -9.186 |
| 2,8-dibromo-1,3-dichlorodibenzo*-p-*dioxin | 4 | -3069.835 | -1.874 | 0.075 | -7.559 |
| 2,8-dibromo-1,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.918 | -1.145 | 0.032 | -7.835 |
| 2,8-dibromo-1,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.931 | -0.870 | 0.044 | -8.676 |
| 2,8-dibromo-1,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.851 | -0.750 | 0.022 | -8.351 |
| 2,8-dibromo-1,9-dichlorodibenzo*-p-*dioxin | 4 | -3069.774 | -2.611 | 0.114 | -7.159 |
| 2,8-dibromo-3,4-dichlorodibenzo*-p-*dioxin | 4 | -3069.865 | -0.488 | 0.034 | -9.166 |
| 2,8-dibromo-3,6-dichlorodibenzo*-p-*dioxin | 4 | -3069.999 | -0.065 | 0.010 | -9.335 |
| 2,8-dibromo-3,7-dichlorodibenzo*-p-*dioxin | 4 | -3069.919 | 0.061 | -0.003 | -9.256 |
| 2,8-dibromo-4,6-dichlorodibenzo*-p-*dioxin | 4 | -3070.071 | 0.652 | -0.025 | -9.798 |
| 1,2,3-tribromo-4-chlorodibenzo*-p-*dioxin | 4 | -3043.171 | -1.439 | 0.091 | -13.829 |
| 1,2,3-tribromo-6-chlorodibenzo*-p-*dioxin | 4 | -3043.366 | -0.892 | 0.068 | -14.252 |
| 1,2,3-tribromo-7-chlorodibenzo*-p-*dioxin | 4 | -3043.450 | -0.598 | 0.042 | -14.129 |
| 1,2,3-tribromo-8-chlorodibenzo*-p-*dioxin | 4 | -3043.448 | -1.875 | 0.073 | -12.467 |
| 1,2,3-tribromo-9-chlorodibenzo*-p-*dioxin | 4 | -3043.357 | -2.856 | 0.127 | -11.991 |
| 1,2,4-tribromo-3-chlorodibenzo*-p-*dioxin | 4 | -3043.072 | -1.517 | 0.097 | -13.852 |
| 1,2,4-tribromo-6-chlorodibenzo*-p-*dioxin | 4 | -3043.359 | -0.292 | 0.052 | -14.997 |
| 1,2,4-tribromo-7-chlorodibenzo*-p-*dioxin | 4 | -3043.450 | 0.046 | 0.012 | -14.594 |
| 1,2,4-tribromo-8-chlorodibenzo*-p-*dioxin | 4 | -3043.450 | -1.225 | 0.027 | -12.528 |
| 1,2,4-tribromo-9-chlorodibenzo*-p-*dioxin | 4 | -3043.359 | -2.202 | 0.078 | -11.982 |
| 1,2,6-tribromo-3-chlorodibenzo*-p-*dioxin | 4 | -3043.283 | -0.915 | 0.068 | -14.223 |
| 1,2,6-tribromo-4-chlorodibenzo*-p-*dioxin | 4 | -3043.363 | -0.243 | 0.056 | -15.194 |
| 1,2,6-tribromo-7-chlorodibenzo*-p-*dioxin | 4 | -3043.311 | 0.002 | 0.003 | -14.301 |
| 1,2,6-tribromo-8-chlorodibenzo*-p-*dioxin | 4 | -3043.463 | -0.921 | 0.047 | -13.632 |
| 1,2,6-tribromo-9-chlorodibenzo*-p-*dioxin | 4 | -3043.380 | -1.785 | 0.103 | -13.432 |
| 1,2,7-tribromo-3-chlorodibenzo*-p-*dioxin | 4 | -3043.358 | -0.614 | 0.044 | -14.167 |
| 1,2,7-tribromo-4-chlorodibenzo*-p-*dioxin | 4 | -3043.445 | 0.097 | 0.008 | -14.590 |
| 1,2,7-tribromo-6-chlorodibenzo*-p-*dioxin | 4 | -3043.310 | 0.030 | -0.002 | -14.226 |
| 1,2,7-tribromo-8-chlorodibenzo*-p-*dioxin | 4 | -3043.376 | -0.789 | 0.017 | -13.124 |
| 1,2,7-tribromo-9-chlorodibenzo*-p-*dioxin | 4 | -3043.447 | -1.500 | 0.071 | -13.139 |
| 1,2,8-tribromo-3-chlorodibenzo*-p-*dioxin | 4 | -3043.356 | -1.846 | 0.073 | -12.540 |
| 1,2,8-tribromo-4-chlorodibenzo*-p-*dioxin | 4 | -3043.444 | -1.122 | 0.032 | -12.858 |
| 1,2,8-tribromo-6-chlorodibenzo*-p-*dioxin | 4 | -3043.455 | -0.838 | 0.041 | -13.638 |
| 1,2,8-tribromo-7-chlorodibenzo*-p-*dioxin | 4 | -3043.375 | -0.725 | 0.018 | -13.274 |
| 1,2,8-tribromo-9-chlorodibenzo*-p-*dioxin | 4 | -3043.298 | -2.584 | 0.104 | -11.930 |
| 1,2,9-tribromo-3-chlorodibenzo*-p-*dioxin | 4 | -3043.274 | -2.770 | 0.129 | -12.224 |
| 1,2,9-tribromo-4-chlorodibenzo*-p-*dioxin | 4 | -3043.362 | -2.038 | 0.083 | -12.428 |
| 1,2,9-tribromo-6-chlorodibenzo*-p-*dioxin | 4 | -3043.379 | -1.672 | 0.091 | -13.339 |
| 1,2,9-tribromo-7-chlorodibenzo*-p-*dioxin | 4 | -3043.454 | -1.364 | 0.071 | -13.401 |
| 1,2,9-tribromo-8-chlorodibenzo*-p-*dioxin | 4 | -3043.300 | -2.510 | 0.115 | -12.358 |
| 1,3,6-tribromo-2-chlorodibenzo*-p-*dioxin | 4 | -3043.187 | -0.930 | 0.084 | -14.627 |
| 1,3,6-tribromo-4-chlorodibenzo*-p-*dioxin | 4 | -3043.278 | 0.512 | 0.014 | -15.579 |
| 1,3,6-tribromo-7-chlorodibenzo*-p-*dioxin | 4 | -3043.371 | 0.913 | -0.035 | -15.063 |
| 1,3,6-tribromo-8-chlorodibenzo*-p-*dioxin | 4 | -3043.523 | -0.010 | 0.008 | -14.368 |
| 1,3,6-tribromo-9-chlorodibenzo*-p-*dioxin | 4 | -3043.441 | -0.872 | 0.071 | -14.354 |
| 1,3,7-tribromo-2-chlorodibenzo*-p-*dioxin | 4 | -3043.262 | -0.630 | 0.048 | -14.258 |
| 1,3,7-tribromo-4-chlorodibenzo*-p-*dioxin | 4 | -3043.360 | 0.850 | -0.006 | -15.697 |
| 1,3,7-tribromo-6-chlorodibenzo*-p-*dioxin | 4 | -3043.370 | 0.937 | -0.037 | -15.058 |
| 1,3,7-tribromo-8-chlorodibenzo*-p-*dioxin | 4 | -3043.437 | 0.127 | -0.019 | -13.948 |
| 1,3,7-tribromo-9-chlorodibenzo*-p-*dioxin | 4 | -3043.509 | -0.587 | 0.029 | -13.801 |
| 1,3,8-tribromo-2-chlorodibenzo*-p-*dioxin | 4 | -3043.261 | -1.859 | 0.081 | -12.741 |
| 1,3,8-tribromo-4-chlorodibenzo*-p-*dioxin | 4 | -3043.360 | -0.369 | 0.020 | -14.017 |
| 1,3,8-tribromo-6-chlorodibenzo*-p-*dioxin | 4 | -3043.516 | 0.068 | 0.005 | -14.442 |
| 1,3,8-tribromo-7-chlorodibenzo*-p-*dioxin | 4 | -3043.437 | 0.188 | -0.014 | -14.196 |
| 1,3,8-tribromo-9-chlorodibenzo*-p-*dioxin | 4 | -3043.362 | -1.655 | 0.076 | -12.986 |
| 1,3,9-tribromo-2-chlorodibenzo*-p-*dioxin | 4 | -3043.179 | -2.790 | 0.136 | -12.385 |
| 1,3,9-tribromo-4-chlorodibenzo*-p-*dioxin | 4 | -3043.278 | -1.286 | 0.070 | -13.559 |
| 1,3,9-tribromo-6-chlorodibenzo*-p-*dioxin | 4 | -3043.441 | -0.763 | 0.054 | -14.123 |
| 1,3,9-tribromo-8-chlorodibenzo*-p-*dioxin | 4 | -3043.364 | -1.579 | 0.077 | -13.158 |
| 1,4,6-tribromo-2-chlorodibenzo*-p-*dioxin | 4 | -3043.278 | -0.337 | 0.065 | -15.263 |
| 1,4,6-tribromo-3-chlorodibenzo*-p-*dioxin | 4 | -3043.278 | 0.445 | 0.033 | -15.943 |
| 1,4,6-tribromo-7-chlorodibenzo*-p-*dioxin | 4 | -3043.296 | 1.727 | -0.086 | -15.326 |
| 1,4,6-tribromo-8-chlorodibenzo*-p-*dioxin | 4 | -3043.449 | 0.796 | -0.051 | -14.407 |
| 1,4,6-tribromo-9-chlorodibenzo*-p-*dioxin | 4 | -3043.366 | -0.068 | 0.010 | -14.338 |
| 1,4,7-tribromo-2-chlorodibenzo*-p-*dioxin | 4 | -3043.360 | -0.005 | 0.016 | -14.616 |
| 1,4,7-tribromo-3-chlorodibenzo*-p-*dioxin | 4 | -3043.359 | 0.777 | -0.003 | -15.634 |
| 1,4,7-tribromo-6-chlorodibenzo*-p-*dioxin | 4 | -3043.294 | 1.742 | -0.079 | -15.537 |
| 1,4,7-tribromo-8-chlorodibenzo*-p-*dioxin | 4 | -3043.368 | 0.968 | -0.087 | -13.820 |
| 1,4,7-tribromo-9-chlorodibenzo*-p-*dioxin | 4 | -3043.441 | 0.252 | -0.038 | -13.695 |
| 1,7,8-tribromo-2-chlorodibenzo*-p-*dioxin | 4 | -3043.376 | -0.771 | 0.020 | -13.237 |
| 1,7,8-tribromo-3-chlorodibenzo*-p-*dioxin | 4 | -3043.529 | 0.161 | -0.019 | -13.996 |
| 1,7,8-tribromo-4-chlorodibenzo*-p-*dioxin | 4 | -3043.454 | 1.060 | -0.082 | -14.112 |
| 1,7,8-tribromo-6-chlorodibenzo*-p-*dioxin | 4 | -3043.283 | 0.975 | -0.065 | -14.421 |
| 1,7,8-tribromo-9-chlorodibenzo*-p-*dioxin | 4 | -3043.275 | -0.383 | 0.008 | -13.694 |
| 2,3,7-tribromo-1-chlorodibenzo*-p-*dioxin | 4 | -3043.359 | -0.668 | 0.046 | -14.114 |
| 2,3,7-tribromo-4-chlorodibenzo*-p-*dioxin | 4 | -3043.357 | 0.719 | 0.007 | -15.782 |
| 2,3,7-tribromo-6-chlorodibenzo*-p-*dioxin | 4 | -3043.375 | 0.786 | -0.028 | -14.999 |
| 2,3,7-tribromo-8-chlorodibenzo*-p-*dioxin | 4 | -3043.443 | -0.022 | 0.001 | -14.178 |
| 2,3,7-tribromo-9-chlorodibenzo*-p-*dioxin | 4 | -3043.522 | -0.776 | 0.049 | -13.953 |
| 1,2,3,4-tetrabromodibenzo*-p-*dioxin | 4 | -3016.693 | -1.521 | 0.096 | -18.779 |
| 1,2,3,6-tetrabromodibenzo*-p-*dioxin | 4 | -3016.807 | -0.935 | 0.086 | -19.630 |
| 1,2,3,7-tetrabromodibenzo*-p-*dioxin | 4 | -3016.882 | -0.632 | 0.048 | -19.215 |
| 1,2,3,8-tetrabromodibenzo*-p-*dioxin | 4 | -3016.881 | -1.858 | 0.073 | -17.495 |
| 1,2,3,9-tetrabromodibenzo*-p-*dioxin | 4 | -3016.798 | -2.782 | 0.129 | -17.180 |
| 1,2,4,6-tetrabromodibenzo*-p-*dioxin | 4 | -3016.801 | -0.328 | 0.065 | -20.259 |
| 1,2,4,7-tetrabromodibenzo*-p-*dioxin | 4 | -3016.883 | 0.009 | 0.016 | -19.622 |
| 1,2,4,8-tetrabromodibenzo*-p-*dioxin | 4 | -3016.882 | -1.208 | 0.030 | -17.634 |
| 1,2,4,9-tetrabromodibenzo*-p-*dioxin | 4 | -3016.800 | -2.125 | 0.078 | -17.124 |
| 1,2,6,7-tetrabromodibenzo*-p-*dioxin | 4 | -3016.835 | 0.000 | 0.001 | -19.224 |
| 1,2,6,8-tetrabromodibenzo*-p-*dioxin | 4 | -3016.895 | -0.905 | 0.056 | -18.892 |
| 1,2,6,9-tetrabromodibenzo*-p-*dioxin | 4 | -3016.819 | -1.716 | 0.101 | -18.508 |
| 1,2,7,8-tetrabromodibenzo*-p-*dioxin | 4 | -3016.899 | -0.760 | 0.020 | -18.237 |
| 1,2,7,9-tetrabromodibenzo*-p-*dioxin | 4 | -3016.886 | -1.408 | 0.075 | -18.416 |
| 1,2,8,9-tetrabromodibenzo*-p-*dioxin | 4 | -3016.823 | -2.495 | 0.113 | -17.314 |
| 1,3,6,8-tetrabromodibenzo*-p-*dioxin | 4 | -3016.955 | 0.001 | 0.010 | -19.437 |
| 1,3,6,9-tetrabromodibenzo*-p-*dioxin | 4 | -3016.881 | -0.806 | 0.060 | -19.190 |
| 1,3,7,8-tetrabromodibenzo*-p-*dioxin | 4 | -3016.961 | 0.150 | -0.020 | -18.945 |
| 1,3,7,9-tetrabromodibenzo*-p-*dioxin | 4 | -3016.949 | -0.497 | 0.027 | -18.918 |
| 1,4,7,8-tetrabromodibenzo*-p-*dioxin | 4 | -3016.892 | 0.992 | -0.081 | -19.001 |
| 1,2,3,4,6-pentachlorodibenzo*-p-*dioxin | 3 | -3363.725 | -0.322 | 0.063 | -1.028 |
| 1,2,3,6,7-pentachlorodibenzo*-p-*dioxin | 3 | -3363.828 | 0.104 | 0.010 | -0.456 |
| 1,2,3,6,8-pentachlorodibenzo*-p-*dioxin | 3 | -3363.958 | -0.820 | 0.047 | 0.393 |
| 1,2,3,6,9-pentachlorodibenzo*-p-*dioxin | 3 | -3363.869 | -1.684 | 0.103 | 0.591 |
| 1,2,3,7,8-pentachlorodibenzo*-p-*dioxin | 3 | -3363.899 | -0.704 | 0.030 | 0.599 |
| 1,2,3,7,9-pentachlorodibenzo*-p-*dioxin | 3 | -3363.949 | -1.391 | 0.076 | 0.742 |
| 1,2,3,8,9-pentachlorodibenzo*-p-*dioxin | 3 | -3363.821 | -2.516 | 0.117 | 1.826 |
| 1,2,4,6,7-pentachlorodibenzo*-p-*dioxin | 3 | -3363.872 | 0.759 | -0.019 | -0.960 |
| 1,2,4,6,8-pentachlorodibenzo*-p-*dioxin | 3 | -3364.000 | -0.163 | 0.010 | 0.092 |
| 1,2,4,7,8-pentachlorodibenzo*-p-*dioxin | 3 | -3363.949 | -0.009 | -0.017 | 0.486 |
| 1,2,4,7,9-pentachlorodibenzo*-p-*dioxin | 3 | -3364.002 | -0.695 | 0.028 | 0.653 |
| 1,2,4,8,9-pentachlorodibenzo*-p-*dioxin | 3 | -3363.872 | -1.800 | 0.060 | 1.933 |
| 1-bromo-2,3,4,6-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.133 | -0.246 | 0.074 | -6.461 |
| 1-bromo-2,3,4,7-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.223 | 0.086 | 0.039 | -6.177 |
| 1-bromo-2,3,4,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.222 | -1.174 | 0.052 | -4.080 |
| 1-bromo-2,3,4,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.133 | -2.143 | 0.102 | -3.523 |
| 1-bromo-2,3,6,7-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.235 | 0.194 | 0.008 | -5.578 |
| 1-bromo-2,3,6,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.364 | -0.731 | 0.042 | -4.650 |
| 1-bromo-2,3,6,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.275 | -1.594 | 0.093 | -4.323 |
| 1-bromo-2,3,7,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.306 | -0.620 | 0.024 | -4.408 |
| 1-bromo-2,3,7,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.357 | -1.305 | 0.067 | -4.191 |
| 1-bromo-2,3,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.227 | -2.433 | 0.106 | -3.049 |
| 1-bromo-2,4,6,7-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.287 | 0.829 | -0.020 | -6.069 |
| 1-bromo-2,4,6,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.413 | -0.095 | 0.010 | -5.038 |
| 1-bromo-2,4,6,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.326 | -0.954 | 0.055 | -4.564 |
| 1-bromo-2,4,7,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.363 | 0.055 | -0.018 | -4.611 |
| 1-bromo-2,4,7,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.416 | -0.628 | 0.023 | -4.346 |
| 1-bromo-2,4,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.285 | -1.737 | 0.057 | -3.110 |
| 1-bromo-2,6,7,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.240 | -0.030 | -0.010 | -4.677 |
| 1-bromo-2,6,7,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.285 | -0.679 | 0.037 | -4.635 |
| 1-bromo-2,6,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.283 | -1.454 | 0.077 | -4.177 |
| 1-bromo-2,7,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.233 | -1.358 | 0.054 | -3.775 |
| 1-bromo-3,4,6,7-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.311 | 1.590 | -0.039 | -7.041 |
| 1-bromo-3,4,6,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.440 | 0.666 | -0.020 | -5.725 |
| 1-bromo-3,4,6,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.351 | -0.199 | 0.032 | -5.420 |
| 1-bromo-3,4,7,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.388 | 0.819 | -0.041 | -5.485 |
| 1-bromo-3,4,7,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.439 | 0.127 | -0.001 | -5.177 |
| 1-bromo-3,4,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.310 | -0.974 | 0.044 | -4.242 |
| 1-bromo-3,6,7,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.393 | 0.884 | -0.055 | -5.246 |
| 1-bromo-3,6,7,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.435 | 0.230 | -0.013 | -5.065 |
| 1-bromo-3,6,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.437 | -0.540 | 0.029 | -4.668 |
| 1-bromo-3,7,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.385 | -0.432 | 0.012 | -4.445 |
| 1-bromo-4,6,7,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.311 | 1.732 | -0.114 | -5.368 |
| 1-bromo-4,6,7,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.356 | 1.076 | -0.067 | -5.312 |
| 1-bromo-4,6,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.355 | 0.309 | -0.030 | -4.791 |
| 1-bromo-4,7,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.311 | 0.456 | -0.056 | -4.408 |
| 1-bromo-6,7,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.165 | 0.369 | -0.030 | -4.943 |
| 2-bromo-1,3,4,6-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.095 | -0.268 | 0.057 | -5.984 |
| 2-bromo-1,3,4,7-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.183 | 0.068 | 0.030 | -5.916 |
| 2-bromo-1,3,4,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.184 | -1.187 | 0.049 | -3.984 |
| 2-bromo-1,3,4,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.094 | -2.152 | 0.096 | -3.357 |
| 2-bromo-1,3,6,7-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.203 | 0.157 | 0.007 | -5.487 |
| 2-bromo-1,3,6,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.333 | -0.765 | 0.042 | -4.590 |
| 2-bromo-1,3,6,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.243 | -1.627 | 0.091 | -4.214 |
| 2-bromo-1,3,7,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.273 | -0.648 | 0.026 | -4.412 |
| 2-bromo-1,3,7,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.323 | -1.331 | 0.071 | -4.251 |
| 2-bromo-1,3,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.195 | -2.457 | 0.105 | -2.983 |
| 2-bromo-1,4,6,7-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.279 | 0.813 | -0.020 | -6.039 |
| 2-bromo-1,4,6,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.408 | -0.106 | 0.006 | -4.914 |
| 2-bromo-1,4,6,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.320 | -0.966 | 0.055 | -4.542 |
| 2-bromo-1,4,7,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.356 | 0.051 | -0.018 | -4.604 |
| 2-bromo-1,4,7,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.408 | -0.633 | 0.022 | -4.312 |
| 2-bromo-1,4,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.278 | -1.738 | 0.056 | -3.084 |
| 2-bromo-1,6,7,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.240 | -0.052 | -0.005 | -4.765 |
| 2-bromo-1,6,7,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.283 | -0.703 | 0.043 | -4.745 |
| 2-bromo-1,6,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.283 | -1.477 | 0.083 | -4.288 |
| 2-bromo-1,7,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.231 | -1.372 | 0.063 | -3.982 |
| 2-bromo-3,4,6,7-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.223 | 1.468 | -0.032 | -7.003 |
| 2-bromo-3,4,6,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.353 | 0.534 | -0.005 | -5.876 |
| 2-bromo-3,4,6,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.271 | -0.367 | 0.038 | -5.267 |
| 2-bromo-3,4,7,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.301 | 0.693 | -0.020 | -5.803 |
| 2-bromo-3,4,7,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.359 | -0.036 | 0.014 | -5.267 |
| 2-bromo-3,4,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.231 | -1.140 | 0.051 | -4.118 |
| 2-bromo-3,6,7,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.306 | 0.738 | -0.039 | -5.396 |
| 2-bromo-3,6,7,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.355 | 0.046 | -0.001 | -5.036 |
| 2-bromo-3,6,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.356 | -0.727 | 0.043 | -4.685 |
| 2-bromo-3,7,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.305 | -0.613 | 0.031 | -4.603 |
| 2-bromo-4,6,7,8-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.379 | 1.441 | -0.073 | -5.857 |
| 2-bromo-4,6,7,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.430 | 0.746 | -0.035 | -5.492 |
| 2-bromo-4,6,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.429 | -0.020 | 0.002 | -4.973 |
| 2-bromo-4,7,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.386 | 0.134 | -0.017 | -4.785 |
| 2-bromo-6,7,8,9-tetrachlorodibenzo*-p-*dioxin | 3 | -3337.246 | 0.028 | -0.001 | -5.022 |
| 1,2-dibromo-3,4,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.619 | -0.245 | 0.058 | -11.033 |
| 1,2-dibromo-3,4,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.708 | 0.088 | 0.029 | -10.907 |
| 1,2-dibromo-3,4,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.708 | -1.166 | 0.047 | -8.951 |
| 1,2-dibromo-3,4,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.618 | -2.131 | 0.098 | -8.428 |
| 1,2-dibromo-3,6,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.724 | 0.190 | 0.008 | -10.556 |
| 1,2-dibromo-3,6,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.854 | -0.729 | 0.040 | -9.587 |
| 1,2-dibromo-3,6,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.764 | -1.589 | 0.089 | -9.214 |
| 1,2-dibromo-3,7,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.794 | -0.618 | 0.024 | -9.397 |
| 1,2-dibromo-3,7,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.844 | -1.299 | 0.065 | -9.136 |
| 1,2-dibromo-3,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.716 | -2.424 | 0.099 | -7.870 |
| 1,2-dibromo-4,6,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.806 | 0.843 | -0.020 | -11.075 |
| 1,2-dibromo-4,6,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.933 | -0.075 | 0.005 | -9.926 |
| 1,2-dibromo-4,6,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.845 | -0.933 | 0.050 | -9.454 |
| 1,2-dibromo-4,7,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.882 | 0.077 | -0.018 | -9.632 |
| 1,2-dibromo-4,7,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.934 | -0.605 | 0.023 | -9.370 |
| 1,2-dibromo-4,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.804 | -1.711 | 0.050 | -7.958 |
| 1,2-dibromo-6,7,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.764 | -0.020 | -0.008 | -9.727 |
| 1,2-dibromo-6,7,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.807 | -0.668 | 0.034 | -9.557 |
| 1,2-dibromo-6,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.806 | -1.440 | 0.075 | -9.131 |
| 1,2-dibromo-7,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.755 | -1.343 | 0.053 | -8.756 |
| 1,3-dibromo-2,4,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.492 | -0.261 | 0.070 | -11.338 |
| 1,3-dibromo-2,4,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.583 | 0.075 | 0.035 | -11.061 |
| 1,3-dibromo-2,4,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.580 | -1.179 | 0.053 | -9.106 |
| 1,3-dibromo-2,4,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.493 | -2.147 | 0.102 | -8.525 |
| 1,3-dibromo-2,6,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.629 | 0.172 | 0.013 | -10.669 |
| 1,3-dibromo-2,6,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.756 | -0.746 | 0.042 | -9.624 |
| 1,3-dibromo-2,6,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.668 | -1.608 | 0.096 | -9.377 |
| 1,3-dibromo-2,7,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.699 | -0.636 | 0.025 | -9.406 |
| 1,3-dibromo-2,7,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.751 | -1.319 | 0.070 | -9.245 |
| 1,3-dibromo-2,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.620 | -2.440 | 0.104 | -7.987 |
| 1,3-dibromo-4,6,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.721 | 1.578 | -0.043 | -11.914 |
| 1,3-dibromo-4,6,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.849 | 0.657 | -0.013 | -10.889 |
| 1,3-dibromo-4,6,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.761 | -0.206 | 0.028 | -10.303 |
| 1,3-dibromo-4,7,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.798 | 0.812 | -0.035 | -10.627 |
| 1,3-dibromo-4,7,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.850 | 0.122 | 0.005 | -10.323 |
| 1,3-dibromo-4,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.720 | -0.976 | 0.042 | -9.186 |
| 1,3-dibromo-6,7,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.824 | 0.871 | -0.056 | -10.191 |
| 1,3-dibromo-6,7,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.868 | 0.218 | -0.013 | -10.038 |
| 1,3-dibromo-6,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.868 | -0.547 | 0.027 | -9.598 |
| 1,3-dibromo-7,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.817 | -0.440 | 0.011 | -9.399 |
| 1,4-dibromo-2,3,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.537 | -0.338 | 0.085 | -11.570 |
| 1,4-dibromo-2,3,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.627 | 0.005 | 0.036 | -10.944 |
| 1,4-dibromo-2,6,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.720 | 0.739 | -0.007 | -11.228 |
| 1,4-dibromo-2,6,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.848 | -0.186 | 0.009 | -9.832 |
| 1,4-dibromo-2,6,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.760 | -1.046 | 0.060 | -9.511 |
| 1,4-dibromo-2,7,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.797 | -0.028 | -0.018 | -9.446 |
| 1,4-dibromo-2,7,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.850 | -0.711 | 0.032 | -9.414 |
| 1,4-dibromo-2,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.720 | -1.822 | 0.050 | -7.760 |
| 1,4-dibromo-6,7,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.750 | 1.659 | -0.108 | -10.377 |
| 1,4-dibromo-6,7,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.794 | 1.001 | -0.068 | -10.136 |
| 1,6-dibromo-2,3,4-trichlorodibenzo*-p-*dioxin | 3 | -3310.574 | -0.292 | 0.068 | -11.211 |
| 1,6-dibromo-2,3,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.649 | 0.119 | 0.010 | -10.485 |
| 1,6-dibromo-2,3,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.800 | -0.794 | 0.048 | -9.679 |
| 1,6-dibromo-2,3,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.719 | -1.642 | 0.100 | -9.406 |
| 1,6-dibromo-2,4,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.700 | 0.751 | -0.019 | -10.943 |
| 1,6-dibromo-2,4,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.850 | -0.161 | 0.011 | -9.932 |
| 1,6-dibromo-2,4,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.770 | -1.005 | 0.063 | -9.666 |
| 1,6-dibromo-2,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.723 | -1.510 | 0.095 | -9.530 |
| 1,6-dibromo-3,4,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.875 | 0.599 | -0.018 | -10.642 |
| 1,6-dibromo-3,4,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.794 | -0.249 | 0.043 | -10.603 |
| 1,7-dibromo-2,3,4-trichlorodibenzo*-p-*dioxin | 3 | -3310.655 | 0.047 | 0.032 | -10.916 |
| 1,7-dibromo-2,3,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.647 | 0.143 | 0.011 | -10.557 |
| 1,7-dibromo-2,3,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.713 | -0.653 | 0.027 | -9.422 |
| 1,7-dibromo-2,3,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.785 | -1.353 | 0.073 | -9.251 |
| 1,7-dibromo-2,4,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.697 | 0.776 | -0.019 | -10.992 |
| 1,7-dibromo-2,4,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.769 | 0.019 | -0.019 | -9.516 |
| 1,7-dibromo-2,4,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.844 | -0.678 | 0.028 | -9.375 |
| 1,7-dibromo-2,6,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.615 | -0.080 | -0.007 | -9.665 |
| 1,7-dibromo-2,6,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.692 | -0.733 | 0.041 | -9.635 |
| 1,7-dibromo-2,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.635 | -1.394 | 0.062 | -8.914 |
| 1,7-dibromo-3,4,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.722 | 1.537 | -0.044 | -11.808 |
| 1,7-dibromo-3,4,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.795 | 0.782 | -0.043 | -10.362 |
| 1,7-dibromo-3,4,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.867 | 0.077 | 0.002 | -10.155 |
| 1,7-dibromo-3,6,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.768 | 0.831 | -0.054 | -10.176 |
| 1,7-dibromo-3,6,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.843 | 0.174 | -0.009 | -10.061 |
| 1,7-dibromo-3,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.788 | -0.472 | 0.016 | -9.472 |
| 1,7-dibromo-4,6,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.686 | 1.676 | -0.112 | -10.318 |
| 1,7-dibromo-4,6,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.762 | 1.018 | -0.070 | -10.123 |
| 1,7-dibromo-4,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.713 | 0.413 | -0.056 | -9.327 |
| 1,7-dibromo-6,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.535 | 0.318 | -0.033 | -9.774 |
| 1,8-dibromo-2,3,4-trichlorodibenzo*-p-*dioxin | 3 | -3310.655 | -1.160 | 0.057 | -9.233 |
| 1,8-dibromo-2,3,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.792 | -0.712 | 0.042 | -9.683 |
| 1,8-dibromo-2,3,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.712 | -0.589 | 0.025 | -9.494 |
| 1,8-dibromo-2,3,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.638 | -2.415 | 0.112 | -8.239 |
| 1,8-dibromo-2,4,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.842 | -0.077 | 0.008 | -10.018 |
| 1,8-dibromo-2,4,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.771 | 0.084 | -0.016 | -9.719 |
| 1,8-dibromo-2,4,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.697 | -1.722 | 0.063 | -8.295 |
| 1,8-dibromo-2,6,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.643 | -0.003 | 0.001 | -10.016 |
| 1,8-dibromo-2,6,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.691 | -1.433 | 0.083 | -9.374 |
| 1,8-dibromo-2,7,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.608 | -1.328 | 0.064 | -9.099 |
| 1,8-dibromo-3,4,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.868 | 0.679 | -0.015 | -10.876 |
| 1,8-dibromo-3,4,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.794 | 0.841 | -0.037 | -10.632 |
| 1,8-dibromo-3,4,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.722 | -0.963 | 0.040 | -9.159 |
| 1,8-dibromo-3,6,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.794 | 0.903 | -0.054 | -10.310 |
| 1,8-dibromo-3,6,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.843 | -0.522 | 0.035 | -9.859 |
| 1,8-dibromo-3,7,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.759 | -0.407 | 0.013 | -9.526 |
| 1,8-dibromo-4,6,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.714 | 1.752 | -0.110 | -10.511 |
| 1,8-dibromo-4,6,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.762 | 0.325 | -0.021 | -10.056 |
| 1,8-dibromo-4,7,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.687 | 0.479 | -0.044 | -9.771 |
| 1,8-dibromo-6,7,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.534 | 0.389 | -0.033 | -9.911 |
| 1,9-dibromo-2,3,4-trichlorodibenzo*-p-*dioxin | 3 | -3310.574 | -2.070 | 0.099 | -8.580 |
| 1,9-dibromo-2,3,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.719 | -1.534 | 0.092 | -9.407 |
| 1,9-dibromo-2,3,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.793 | -1.216 | 0.067 | -9.358 |
| 1,9-dibromo-2,3,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.641 | -2.346 | 0.111 | -8.346 |
| 1,9-dibromo-2,4,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.769 | -0.893 | 0.054 | -9.649 |
| 1,9-dibromo-2,4,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.852 | -0.539 | 0.021 | -9.461 |
| 1,9-dibromo-2,4,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.698 | -1.648 | 0.062 | -8.412 |
| 1,9-dibromo-2,6,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.724 | -0.603 | 0.036 | -9.751 |
| 1,9-dibromo-3,4,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.795 | -0.136 | 0.026 | -10.380 |
| 1,9-dibromo-3,4,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.875 | 0.218 | -0.007 | -10.192 |
| 2,3-dibromo-1,4,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.584 | -0.297 | 0.058 | -10.939 |
| 2,3-dibromo-1,4,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.673 | 0.043 | 0.027 | -10.775 |
| 2,3-dibromo-1,6,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.724 | 0.126 | 0.009 | -10.458 |
| 2,3-dibromo-1,6,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.854 | -0.791 | 0.044 | -9.571 |
| 2,3-dibromo-1,6,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.765 | -1.652 | 0.094 | -9.222 |
| 2,3-dibromo-1,7,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.795 | -0.673 | 0.027 | -9.368 |
| 2,3-dibromo-1,7,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.846 | -1.356 | 0.070 | -9.156 |
| 2,3-dibromo-1,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.717 | -2.475 | 0.106 | -7.953 |
| 2,3-dibromo-6,7,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.829 | 0.712 | -0.038 | -10.350 |
| 2,3-dibromo-6,7,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.879 | 0.022 | 0.003 | -10.072 |
| 2,7-dibromo-1,3,4-trichlorodibenzo*-p-*dioxin | 3 | -3310.615 | 0.029 | 0.033 | -10.914 |
| 2,7-dibromo-1,3,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.615 | 0.105 | 0.008 | -10.412 |
| 2,7-dibromo-1,3,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.681 | -0.682 | 0.029 | -9.424 |
| 2,7-dibromo-1,3,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.752 | -1.381 | 0.075 | -9.255 |
| 2,7-dibromo-1,4,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.690 | 0.760 | -0.018 | -10.988 |
| 2,7-dibromo-1,4,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.763 | 0.013 | -0.018 | -9.531 |
| 2,7-dibromo-1,4,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.836 | -0.684 | 0.028 | -9.365 |
| 2,7-dibromo-1,8,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.635 | -1.410 | 0.071 | -9.117 |
| 2,7-dibromo-3,4,8-trichlorodibenzo*-p-*dioxin | 3 | -3310.708 | 0.654 | -0.020 | -10.728 |
| 2,7-dibromo-3,4,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.787 | -0.090 | 0.017 | -10.237 |
| 2,8-dibromo-1,3,4-trichlorodibenzo*-p-*dioxin | 3 | -3310.616 | -1.174 | 0.049 | -9.005 |
| 2,8-dibromo-1,3,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.761 | -0.747 | 0.042 | -9.621 |
| 2,8-dibromo-1,3,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.679 | -0.618 | 0.025 | -9.444 |
| 2,8-dibromo-1,4,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.836 | -0.090 | 0.006 | -9.942 |
| 2,8-dibromo-1,4,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.763 | 0.079 | -0.017 | -9.685 |
| 2,8-dibromo-1,4,9-trichlorodibenzo*-p-*dioxin | 3 | -3310.690 | -1.724 | 0.056 | -8.110 |
| 2,8-dibromo-1,6,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.642 | -0.027 | -0.003 | -9.866 |
| 2,8-dibromo-3,4,6-trichlorodibenzo*-p-*dioxin | 3 | -3310.782 | 0.547 | -0.006 | -10.871 |
| 2,8-dibromo-3,4,7-trichlorodibenzo*-p-*dioxin | 3 | -3310.708 | 0.715 | -0.022 | -10.794 |
| 1,2,3-tribromo-4,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.110 | -0.262 | 0.063 | -16.115 |
| 1,2,3-tribromo-4,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.200 | 0.075 | 0.029 | -15.866 |
| 1,2,3-tribromo-4,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.199 | -1.175 | 0.047 | -13.919 |
| 1,2,3-tribromo-4,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.110 | -2.139 | 0.094 | -13.293 |
| 1,2,3-tribromo-6,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.248 | 0.168 | 0.009 | -15.518 |
| 1,2,3-tribromo-6,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.376 | -0.746 | 0.040 | -14.533 |
| 1,2,3-tribromo-6,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.287 | -1.605 | 0.089 | -14.162 |
| 1,2,3-tribromo-7,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.318 | -0.634 | 0.024 | -14.344 |
| 1,2,3-tribromo-7,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.369 | -1.314 | 0.067 | -14.138 |
| 1,2,3-tribromo-8,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.239 | -2.434 | 0.098 | -12.803 |
| 1,2,4-tribromo-3,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.013 | -0.339 | 0.069 | -16.140 |
| 1,2,4-tribromo-3,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.102 | 0.005 | 0.036 | -15.931 |
| 1,2,4-tribromo-3,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.103 | -1.252 | 0.047 | -13.788 |
| 1,2,4-tribromo-3,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.012 | -2.218 | 0.094 | -13.159 |
| 1,2,4-tribromo-6,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.243 | 0.752 | -0.008 | -16.206 |
| 1,2,4-tribromo-6,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.372 | -0.168 | 0.007 | -14.793 |
| 1,2,4-tribromo-6,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.283 | -1.027 | 0.056 | -14.423 |
| 1,2,4-tribromo-7,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.371 | -0.690 | 0.024 | -14.226 |
| 1,2,4-tribromo-8,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.242 | -1.798 | 0.047 | -12.707 |
| 1,2,6-tribromo-3,4-dichlorodibenzo*-p-*dioxin | 3 | -3284.060 | -0.292 | 0.070 | -16.248 |
| 1,2,6-tribromo-3,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.137 | 0.113 | 0.008 | -15.406 |
| 1,2,6-tribromo-3,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.290 | -0.795 | 0.045 | -14.584 |
| 1,2,6-tribromo-3,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.207 | -1.639 | 0.094 | -14.241 |
| 1,2,6-tribromo-4,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.219 | 0.764 | -0.019 | -15.948 |
| 1,2,6-tribromo-4,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.370 | -0.143 | 0.007 | -14.842 |
| 1,2,6-tribromo-4,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.289 | -0.986 | 0.056 | -14.501 |
| 1,2,6-tribromo-7,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.172 | -0.110 | 0.000 | -14.761 |
| 1,2,6-tribromo-7,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.222 | -0.739 | 0.044 | -14.679 |
| 1,2,6-tribromo-8,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.246 | -1.498 | 0.089 | -14.376 |
| 1,2,7-tribromo-3,4-dichlorodibenzo*-p-*dioxin | 3 | -3284.140 | 0.050 | 0.038 | -16.063 |
| 1,2,7-tribromo-3,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.137 | 0.140 | 0.012 | -15.562 |
| 1,2,7-tribromo-3,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.202 | -0.650 | 0.025 | -14.361 |
| 1,2,7-tribromo-3,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.273 | -1.347 | 0.070 | -14.170 |
| 1,2,7-tribromo-4,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.217 | 0.791 | -0.015 | -16.104 |
| 1,2,7-tribromo-4,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.289 | 0.041 | -0.018 | -14.564 |
| 1,2,7-tribromo-4,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.362 | -0.655 | 0.026 | -14.347 |
| 1,2,7-tribromo-6,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.139 | -0.070 | -0.006 | -14.689 |
| 1,2,7-tribromo-6,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.214 | -0.722 | 0.038 | -14.557 |
| 1,2,7-tribromo-8,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.158 | -1.378 | 0.061 | -13.898 |
| 1,2,8-tribromo-3,4-dichlorodibenzo*-p-*dioxin | 3 | -3284.140 | -1.152 | 0.047 | -13.974 |
| 1,2,8-tribromo-3,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.281 | -0.711 | 0.039 | -14.592 |
| 1,2,8-tribromo-3,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.200 | -0.587 | 0.024 | -14.457 |
| 1,2,8-tribromo-3,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.126 | -2.406 | 0.100 | -12.930 |
| 1,2,8-tribromo-4,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.362 | -0.057 | 0.007 | -15.010 |
| 1,2,8-tribromo-4,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.289 | 0.105 | -0.018 | -14.687 |
| 1,2,8-tribromo-4,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.216 | -1.696 | 0.055 | -13.117 |
| 1,2,8-tribromo-6,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.166 | 0.006 | -0.008 | -14.779 |
| 1,2,8-tribromo-6,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.213 | -1.419 | 0.076 | -14.198 |
| 1,2,8-tribromo-7,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.130 | -1.313 | 0.056 | -13.899 |
| 1,2,9-tribromo-3,4-dichlorodibenzo*-p-*dioxin | 3 | -3284.059 | -2.056 | 0.092 | -13.411 |
| 1,2,9-tribromo-3,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.208 | -1.527 | 0.084 | -14.198 |
| 1,2,9-tribromo-3,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.281 | -1.209 | 0.063 | -14.253 |
| 1,2,9-tribromo-3,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.130 | -2.335 | 0.105 | -13.197 |
| 1,2,9-tribromo-4,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.289 | -0.870 | 0.047 | -14.491 |
| 1,2,9-tribromo-4,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.370 | -0.514 | 0.022 | -14.515 |
| 1,2,9-tribromo-4,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.217 | -1.621 | 0.057 | -13.313 |
| 1,2,9-tribromo-6,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.246 | -0.590 | 0.035 | -14.729 |
| 1,2,9-tribromo-6,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.221 | -1.367 | 0.076 | -14.297 |
| 1,2,9-tribromo-7,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.163 | -1.249 | 0.060 | -14.120 |
| 1,3,6-tribromo-2,4-dichlorodibenzo*-p-*dioxin | 3 | -3283.933 | -0.307 | 0.065 | -16.113 |
| 1,3,6-tribromo-2,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.042 | 0.096 | 0.020 | -15.703 |
| 1,3,6-tribromo-2,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.192 | -0.811 | 0.048 | -14.649 |
| 1,3,6-tribromo-2,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.112 | -1.658 | 0.104 | -14.482 |
| 1,3,6-tribromo-4,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.134 | 1.500 | -0.051 | -16.555 |
| 1,3,6-tribromo-4,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.285 | 0.590 | -0.016 | -15.677 |
| 1,3,6-tribromo-4,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.204 | -0.257 | 0.041 | -15.536 |
| 1,3,6-tribromo-7,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.232 | 0.780 | -0.046 | -15.275 |
| 1,3,6-tribromo-7,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.282 | 0.149 | 0.001 | -15.267 |
| 1,3,6-tribromo-8,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.307 | -0.606 | 0.043 | -14.894 |
| 1,3,7-tribromo-2,4-dichlorodibenzo*-p-*dioxin | 3 | -3284.014 | 0.037 | 0.039 | -16.088 |
| 1,3,7-tribromo-2,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.040 | 0.121 | 0.013 | -15.570 |
| 1,3,7-tribromo-2,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.105 | -0.668 | 0.028 | -14.423 |
| 1,3,7-tribromo-2,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.179 | -1.367 | 0.075 | -14.279 |
| 1,3,7-tribromo-4,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.132 | 1.524 | -0.048 | -16.679 |
| 1,3,7-tribromo-4,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.204 | 0.774 | -0.044 | -15.321 |
| 1,3,7-tribromo-4,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.278 | 0.071 | 0.000 | -15.091 |
| 1,3,7-tribromo-6,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.199 | 0.817 | -0.054 | -15.145 |
| 1,3,7-tribromo-6,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.275 | 0.162 | -0.010 | -15.008 |
| 1,3,7-tribromo-8,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.220 | -0.479 | 0.014 | -14.403 |
| 1,3,8-tribromo-2,4-dichlorodibenzo*-p-*dioxin | 3 | -3284.013 | -1.165 | 0.055 | -14.181 |
| 1,3,8-tribromo-2,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.184 | -0.728 | 0.041 | -14.629 |
| 1,3,8-tribromo-2,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.106 | -0.605 | 0.023 | -14.414 |
| 1,3,8-tribromo-2,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.032 | -2.423 | 0.108 | -13.123 |
| 1,3,8-tribromo-4,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.277 | 0.670 | -0.014 | -15.885 |
| 1,3,8-tribromo-4,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.205 | 0.835 | -0.038 | -15.594 |
| 1,3,8-tribromo-4,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.132 | -0.964 | 0.038 | -14.105 |
| 1,3,8-tribromo-6,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.226 | 0.890 | -0.054 | -15.281 |
| 1,3,8-tribromo-6,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.274 | -0.530 | 0.034 | -14.813 |
| 1,3,8-tribromo-7,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.192 | -0.416 | 0.012 | -14.478 |
| 1,3,9-tribromo-2,4-dichlorodibenzo*-p-*dioxin | 3 | -3283.934 | -2.075 | 0.100 | -13.606 |
| 1,3,9-tribromo-2,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.112 | -1.550 | 0.092 | -14.379 |
| 1,3,9-tribromo-2,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.187 | -1.232 | 0.067 | -14.330 |
| 1,3,9-tribromo-2,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.034 | -2.354 | 0.111 | -13.334 |
| 1,3,9-tribromo-4,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.204 | -0.144 | 0.027 | -15.390 |
| 1,3,9-tribromo-4,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.286 | 0.212 | -0.007 | -15.180 |
| 1,3,9-tribromo-4,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.134 | -0.886 | 0.043 | -14.386 |
| 1,3,9-tribromo-6,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.307 | 0.294 | -0.016 | -15.101 |
| 1,3,9-tribromo-6,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.283 | -0.475 | 0.030 | -14.814 |
| 1,3,9-tribromo-7,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.225 | -0.348 | 0.014 | -14.655 |
| 1,4,6-tribromo-2,3-dichlorodibenzo*-p-*dioxin | 3 | -3283.979 | -0.372 | 0.080 | -16.369 |
| 1,4,6-tribromo-2,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.135 | 0.672 | -0.012 | -15.967 |
| 1,4,6-tribromo-2,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.285 | -0.241 | 0.010 | -14.746 |
| 1,4,6-tribromo-2,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.205 | -1.085 | 0.068 | -14.637 |
| 1,4,6-tribromo-3,7-dichlorodibenzo*-p-*dioxin | 3 | -3284.134 | 1.441 | -0.032 | -16.934 |
| 1,4,6-tribromo-3,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.287 | 0.525 | -0.007 | -15.785 |
| 1,4,6-tribromo-3,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.204 | -0.325 | 0.052 | -15.690 |
| 1,4,6-tribromo-7,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.159 | 1.578 | -0.110 | -15.169 |
| 1,4,6-tribromo-7,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.209 | 0.940 | -0.068 | -15.017 |
| 1,4,6-tribromo-8,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.234 | 0.184 | -0.015 | -14.928 |
| 1,4,7-tribromo-2,3-dichlorodibenzo*-p-*dioxin | 3 | -3284.059 | -0.035 | 0.039 | -15.940 |
| 1,4,7-tribromo-2,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.131 | 0.685 | -0.008 | -16.097 |
| 1,4,7-tribromo-2,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.204 | -0.065 | -0.018 | -14.375 |
| 1,4,7-tribromo-2,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.278 | -0.762 | 0.028 | -14.209 |
| 1,4,7-tribromo-3,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.132 | 1.453 | -0.032 | -16.958 |
| 1,4,7-tribromo-3,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.205 | 0.705 | -0.038 | -15.343 |
| 1,4,7-tribromo-3,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.277 | -0.001 | 0.004 | -15.056 |
| 1,4,7-tribromo-6,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.125 | 1.601 | -0.111 | -15.194 |
| 1,4,7-tribromo-6,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.201 | 0.941 | -0.065 | -15.099 |
| 1,4,7-tribromo-8,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.152 | 0.344 | -0.061 | -14.058 |
| 1,7,8-tribromo-2,3-dichlorodibenzo*-p-*dioxin | 3 | -3284.236 | -0.626 | 0.028 | -14.479 |
| 1,7,8-tribromo-2,4-dichlorodibenzo*-p-*dioxin | 3 | -3284.293 | 0.044 | -0.017 | -14.594 |
| 1,7,8-tribromo-2,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.137 | -0.048 | -0.004 | -14.784 |
| 1,7,8-tribromo-2,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.130 | -1.366 | 0.063 | -13.978 |
| 1,7,8-tribromo-3,4-dichlorodibenzo*-p-*dioxin | 3 | -3284.318 | 0.801 | -0.036 | -15.559 |
| 1,7,8-tribromo-3,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.289 | 0.857 | -0.054 | -15.205 |
| 1,7,8-tribromo-3,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.281 | -0.447 | 0.015 | -14.479 |
| 1,7,8-tribromo-4,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.208 | 1.702 | -0.110 | -15.399 |
| 1,7,8-tribromo-4,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.208 | 0.436 | -0.054 | -14.407 |
| 1,7,8-tribromo-6,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.024 | 0.348 | -0.027 | -14.973 |
| 2,3,7-tribromo-1,4-dichlorodibenzo*-p-*dioxin | 3 | -3284.105 | 0.003 | 0.029 | -15.745 |
| 2,3,7-tribromo-1,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.136 | 0.074 | 0.011 | -15.409 |
| 2,3,7-tribromo-1,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.202 | -0.707 | 0.030 | -14.381 |
| 2,3,7-tribromo-1,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.275 | -1.406 | 0.077 | -14.237 |
| 2,3,7-tribromo-4,6-dichlorodibenzo*-p-*dioxin | 3 | -3284.128 | 1.383 | -0.030 | -16.875 |
| 2,3,7-tribromo-4,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.201 | 0.632 | -0.021 | -15.644 |
| 2,3,7-tribromo-4,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.281 | -0.109 | 0.018 | -15.210 |
| 2,3,7-tribromo-6,8-dichlorodibenzo*-p-*dioxin | 3 | -3284.203 | 0.656 | -0.035 | -15.326 |
| 2,3,7-tribromo-6,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.286 | -0.038 | 0.003 | -14.957 |
| 2,3,7-tribromo-8,9-dichlorodibenzo*-p-*dioxin | 3 | -3284.231 | -0.672 | 0.037 | -14.625 |
| 1,2,3,4-tetrabromo-6-chlorodibenzo*-p-*dioxin | 3 | -3257.632 | -0.350 | 0.072 | -21.157 |
| 1,2,3,4-tetrabromo-7-chlorodibenzo*-p-*dioxin | 3 | -3257.722 | -0.006 | 0.036 | -20.870 |
| 1,2,3,6-tetrabromo-4-chlorodibenzo*-p-*dioxin | 3 | -3257.552 | -0.311 | 0.068 | -21.144 |
| 1,2,3,6-tetrabromo-7-chlorodibenzo*-p-*dioxin | 3 | -3257.661 | 0.091 | 0.010 | -20.394 |
| 1,2,3,6-tetrabromo-8-chlorodibenzo*-p-*dioxin | 3 | -3257.812 | -0.812 | 0.045 | -19.530 |
| 1,2,3,6-tetrabromo-9-chlorodibenzo*-p-*dioxin | 3 | -3257.731 | -1.656 | 0.096 | -19.239 |
| 1,2,3,7-tetrabromo-4-chlorodibenzo*-p-*dioxin | 3 | -3257.632 | 0.037 | 0.034 | -20.919 |
| 1,2,3,7-tetrabromo-6-chlorodibenzo*-p-*dioxin | 3 | -3257.660 | 0.118 | 0.013 | -20.525 |
| 1,2,3,7-tetrabromo-8-chlorodibenzo*-p-*dioxin | 3 | -3257.725 | -0.666 | 0.026 | -19.335 |
| 1,2,3,7-tetrabromo-9-chlorodibenzo*-p-*dioxin | 3 | -3257.798 | -1.363 | 0.071 | -19.143 |
| 1,2,3,8-tetrabromo-4-chlorodibenzo*-p-*dioxin | 3 | -3257.632 | -1.161 | 0.048 | -18.967 |
| 1,2,3,8-tetrabromo-6-chlorodibenzo*-p-*dioxin | 3 | -3257.804 | -0.727 | 0.041 | -19.592 |
| 1,2,3,8-tetrabromo-7-chlorodibenzo*-p-*dioxin | 3 | -3257.725 | -0.603 | 0.025 | -19.431 |
| 1,2,3,8-tetrabromo-9-chlorodibenzo*-p-*dioxin | 3 | -3257.651 | -2.416 | 0.100 | -17.889 |
| 1,2,3,9-tetrabromo-4-chlorodibenzo*-p-*dioxin | 3 | -3257.551 | -2.065 | 0.092 | -18.378 |
| 1,2,3,9-tetrabromo-6-chlorodibenzo*-p-*dioxin | 3 | -3257.731 | -1.544 | 0.085 | -19.170 |
| 1,2,3,9-tetrabromo-7-chlorodibenzo*-p-*dioxin | 3 | -3257.805 | -1.225 | 0.064 | -19.227 |
| 1,2,3,9-tetrabromo-8-chlorodibenzo*-p-*dioxin | 3 | -3257.653 | -2.346 | 0.106 | -18.180 |
| 1,2,4,6-tetrabromo-3-chlorodibenzo*-p-*dioxin | 3 | -3257.455 | -0.375 | 0.081 | -21.376 |
| 1,2,4,6-tetrabromo-7-chlorodibenzo*-p-*dioxin | 3 | -3257.657 | 0.683 | -0.012 | -20.967 |
| 1,2,4,6-tetrabromo-8-chlorodibenzo*-p-*dioxin | 3 | -3257.808 | -0.225 | 0.010 | -19.756 |
| 1,2,4,6-tetrabromo-9-chlorodibenzo*-p-*dioxin | 3 | -3257.727 | -1.068 | 0.061 | -19.467 |
| 1,2,4,7-tetrabromo-3-chlorodibenzo*-p-*dioxin | 3 | -3257.534 | -0.034 | 0.039 | -20.930 |
| 1,2,4,7-tetrabromo-6-chlorodibenzo*-p-*dioxin | 3 | -3257.655 | 0.698 | -0.007 | -21.127 |
| 1,2,4,7-tetrabromo-8-chlorodibenzo*-p-*dioxin | 3 | -3257.727 | -0.045 | -0.018 | -19.392 |
| 1,2,4,7-tetrabromo-9-chlorodibenzo*-p-*dioxin | 3 | -3257.799 | -0.741 | 0.026 | -19.176 |
| 1,2,4,8-tetrabromo-3-chlorodibenzo*-p-*dioxin | 3 | -3257.534 | -1.237 | 0.048 | -18.839 |
| 1,2,4,8-tetrabromo-6-chlorodibenzo*-p-*dioxin | 3 | -3257.800 | -0.150 | 0.009 | -19.876 |
| 1,2,4,8-tetrabromo-7-chlorodibenzo*-p-*dioxin | 3 | -3257.727 | 0.021 | -0.017 | -19.546 |
| 1,2,4,8-tetrabromo-9-chlorodibenzo*-p-*dioxin | 3 | -3257.654 | -1.782 | 0.048 | -17.763 |
| 1,2,4,9-tetrabromo-3-chlorodibenzo*-p-*dioxin | 3 | -3257.454 | -2.143 | 0.093 | -18.272 |
| 1,2,4,9-tetrabromo-6-chlorodibenzo*-p-*dioxin | 3 | -3257.727 | -0.964 | 0.051 | -19.408 |
| 1,2,4,9-tetrabromo-7-chlorodibenzo*-p-*dioxin | 3 | -3257.808 | -0.599 | 0.020 | -19.293 |
| 1,2,4,9-tetrabromo-8-chlorodibenzo*-p-*dioxin | 3 | -3257.656 | -1.708 | 0.051 | -17.984 |
| 1,2,6,7-tetrabromo-3-chlorodibenzo*-p-*dioxin | 3 | -3257.661 | 0.105 | 0.009 | -20.395 |
| 1,2,6,7-tetrabromo-4-chlorodibenzo*-p-*dioxin | 3 | -3257.741 | 0.753 | -0.020 | -20.879 |
| 1,2,6,8-tetrabromo-3-chlorodibenzo*-p-*dioxin | 3 | -3257.720 | -0.781 | 0.046 | -19.633 |
| 1,2,6,8-tetrabromo-4-chlorodibenzo*-p-*dioxin | 3 | -3257.802 | -0.130 | 0.010 | -19.941 |
| 1,2,6,8-tetrabromo-7-chlorodibenzo*-p-*dioxin | 3 | -3257.565 | -0.087 | 0.010 | -20.068 |
| 1,2,6,8-tetrabromo-9-chlorodibenzo*-p-*dioxin | 3 | -3257.656 | -1.485 | 0.090 | -19.427 |
| 1,2,6,9-tetrabromo-3-chlorodibenzo*-p-*dioxin | 3 | -3257.647 | -1.574 | 0.092 | -19.309 |
| 1,2,6,9-tetrabromo-4-chlorodibenzo*-p-*dioxin | 3 | -3257.728 | -0.919 | 0.052 | -19.521 |
| 1,2,6,9-tetrabromo-7-chlorodibenzo*-p-*dioxin | 3 | -3257.657 | -0.658 | 0.041 | -19.753 |
| 1,2,6,9-tetrabromo-8-chlorodibenzo*-p-*dioxin | 3 | -3257.657 | -1.424 | 0.093 | -19.623 |
| 1,2,7,8-tetrabromo-3-chlorodibenzo*-p-*dioxin | 3 | -3257.725 | -0.624 | 0.027 | -19.442 |
| 1,2,7,8-tetrabromo-4-chlorodibenzo*-p-*dioxin | 3 | -3257.812 | 0.066 | -0.018 | -19.590 |
| 1,2,7,8-tetrabromo-6-chlorodibenzo*-p-*dioxin | 3 | -3257.660 | -0.038 | -0.006 | -19.730 |
| 1,2,7,8-tetrabromo-9-chlorodibenzo*-p-*dioxin | 3 | -3257.652 | -1.349 | 0.061 | -18.938 |
| 1,2,7,9-tetrabromo-3-chlorodibenzo*-p-*dioxin | 3 | -3257.713 | -1.256 | 0.069 | -19.314 |
| 1,2,7,9-tetrabromo-4-chlorodibenzo*-p-*dioxin | 3 | -3257.801 | -0.564 | 0.024 | -19.466 |
| 1,2,7,9-tetrabromo-6-chlorodibenzo*-p-*dioxin | 3 | -3257.656 | -0.645 | 0.040 | -19.752 |
| 1,2,7,9-tetrabromo-8-chlorodibenzo*-p-*dioxin | 3 | -3257.556 | -1.283 | 0.065 | -19.187 |
| 1,2,8,9-tetrabromo-3-chlorodibenzo*-p-*dioxin | 3 | -3257.651 | -2.320 | 0.104 | -18.179 |
| 1,2,8,9-tetrabromo-4-chlorodibenzo*-p-*dioxin | 3 | -3257.740 | -1.610 | 0.058 | -18.339 |
| 1,3,6,8-tetrabromo-2-chlorodibenzo*-p-*dioxin | 3 | -3257.624 | -0.797 | 0.046 | -19.620 |
| 1,3,6,8-tetrabromo-4-chlorodibenzo*-p-*dioxin | 3 | -3257.717 | 0.598 | -0.015 | -20.714 |
| 1,3,6,9-tetrabromo-2-chlorodibenzo*-p-*dioxin | 3 | -3257.552 | -1.595 | 0.100 | -19.494 |
| 1,3,6,9-tetrabromo-4-chlorodibenzo*-p-*dioxin | 3 | -3257.644 | -0.192 | 0.037 | -20.552 |
| 1,3,6,9-tetrabromo-7-chlorodibenzo*-p-*dioxin | 3 | -3257.717 | 0.227 | -0.013 | -20.049 |
| 1,3,6,9-tetrabromo-8-chlorodibenzo*-p-*dioxin | 3 | -3257.718 | -0.533 | 0.038 | -19.905 |
| 1,3,7,8-tetrabromo-2-chlorodibenzo*-p-*dioxin | 3 | -3257.629 | -0.642 | 0.028 | -19.451 |
| 1,3,7,8-tetrabromo-4-chlorodibenzo*-p-*dioxin | 3 | -3257.728 | 0.794 | -0.042 | -20.390 |
| 1,3,7,8-tetrabromo-6-chlorodibenzo*-p-*dioxin | 3 | -3257.720 | 0.844 | -0.054 | -20.176 |
| 1,3,7,8-tetrabromo-9-chlorodibenzo*-p-*dioxin | 3 | -3257.713 | -0.455 | 0.014 | -19.433 |
| 1,3,7,9-tetrabromo-2-chlorodibenzo*-p-*dioxin | 3 | -3257.618 | -1.279 | 0.072 | -19.365 |
| 1,3,7,9-tetrabromo-4-chlorodibenzo*-p-*dioxin | 3 | -3257.717 | 0.161 | -0.005 | -20.129 |
| 1,4,6,9-tetrabromo-2-chlorodibenzo*-p-*dioxin | 3 | -3257.645 | -1.021 | 0.068 | -19.755 |
| 1,4,7,8-tetrabromo-2-chlorodibenzo*-p-*dioxin | 3 | -3257.728 | -0.039 | -0.017 | -19.429 |
| 1,4,7,8-tetrabromo-6-chlorodibenzo*-p-*dioxin | 3 | -3257.647 | 1.628 | -0.105 | -20.380 |
| 2,3,7,8-tetrabromo-1-chlorodibenzo*-p-*dioxin | 3 | -3257.725 | -0.682 | 0.029 | -19.382 |
| 1,2,3,4,6-pentabromodibenzo*-p-*dioxin | 3 | -3231.074 | -0.388 | 0.078 | -26.234 |
| 1,2,3,4,7-pentabromodibenzo*-p-*dioxin | 3 | -3231.154 | -0.046 | 0.039 | -25.867 |
| 1,2,3,6,7-pentabromodibenzo*-p-*dioxin | 3 | -3231.184 | 0.083 | 0.011 | -25.383 |
| 1,2,3,6,8-pentabromodibenzo*-p-*dioxin | 3 | -3231.244 | -0.798 | 0.046 | -24.579 |
| 1,2,3,6,9-pentabromodibenzo*-p-*dioxin | 3 | -3231.171 | -1.591 | 0.093 | -24.281 |
| 1,2,3,7,8-pentabromodibenzo*-p-*dioxin | 3 | -3231.248 | -0.640 | 0.026 | -24.364 |
| 1,2,3,7,9-pentabromodibenzo*-p-*dioxin | 3 | -3231.237 | -1.272 | 0.071 | -24.313 |
| 1,2,3,8,9-pentabromodibenzo*-p-*dioxin | 3 | -3231.175 | -2.332 | 0.104 | -23.134 |
| 1,2,4,6,7-pentabromodibenzo*-p-*dioxin | 3 | -3231.180 | 0.671 | -0.012 | -25.923 |
| 1,2,4,6,8-pentabromodibenzo*-p-*dioxin | 3 | -3231.240 | -0.211 | 0.010 | -24.779 |
| 1,2,4,6,9-pentabromodibenzo*-p-*dioxin | 3 | -3231.167 | -1.002 | 0.057 | -24.485 |
| 1,2,4,7,9-pentabromodibenzo*-p-*dioxin | 3 | -3231.239 | -0.649 | 0.025 | -24.322 |
| 1,2,4,8,9-pentabromodibenzo*-p-*dioxin | 3 | -3231.178 | -1.696 | 0.052 | -23.012 |
| 1,2,3,4,6,7-hexachlorodibenzo*-p-*dioxin | 2 | -3604.606 | 0.703 | 0.002 | -2.175 |
| 1,2,3,4,7,8-hexachlorodibenzo*-p-*dioxin | 2 | -3604.681 | -0.047 | 0.003 | -0.738 |
| 1,2,3,6,7,8-hexachlorodibenzo*-p-*dioxin | 2 | -3604.692 | 0.000 | 0.000 | -0.749 |
| 1,2,3,6,7,9-hexachlorodibenzo*-p-*dioxin | 2 | -3604.736 | -0.638 | 0.041 | -0.573 |
| 1,2,3,6,8,9-hexachlorodibenzo*-p-*dioxin | 2 | -3604.736 | -1.399 | 0.080 | -0.115 |
| 1,2,3,7,8,9-hexachlorodibenzo*-p-*dioxin | 2 | -3604.685 | -1.284 | 0.063 | 0.095 |
| 1,2,4,6,7,9-hexachlorodibenzo*-p-*dioxin | 2 | -3604.781 | 0.000 | 0.003 | -0.810 |
| 1,2,4,6,8,9-hexachlorodibenzo*-p-*dioxin | 2 | -3604.780 | -0.752 | 0.033 | -0.136 |
| 1-bromo-2,3,4,6,7-pentachlorodibenzo*-p-*dioxin | 2 | -3578.015 | 0.783 | 0.000 | -7.278 |
| 1-bromo-2,3,4,6,8-pentachlorodibenzo*-p-*dioxin | 2 | -3578.142 | -0.128 | 0.024 | -6.117 |
| 1-bromo-2,3,4,6,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.055 | -0.978 | 0.069 | -5.660 |
| 1-bromo-2,3,4,7,8-pentachlorodibenzo*-p-*dioxin | 2 | -3578.091 | 0.027 | 0.001 | -5.829 |
| 1-bromo-2,3,4,7,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.143 | -0.647 | 0.039 | -5.504 |
| 1-bromo-2,3,4,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.014 | -1.744 | 0.068 | -4.161 |
| 1-bromo-2,3,6,7,8-pentachlorodibenzo*-p-*dioxin | 2 | -3578.099 | 0.092 | -0.004 | -5.823 |
| 1-bromo-2,3,6,7,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.143 | -0.543 | 0.035 | -5.601 |
| 1-bromo-2,3,6,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.143 | -1.305 | 0.072 | -5.089 |
| 1-bromo-2,3,7,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.092 | -1.196 | 0.056 | -4.894 |
| 1-bromo-2,4,6,7,8-pentachlorodibenzo*-p-*dioxin | 2 | -3578.150 | 0.710 | -0.039 | -6.099 |
| 1-bromo-2,4,6,7,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.196 | 0.075 | -0.002 | -5.824 |
| 1-bromo-2,4,6,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.193 | -0.679 | 0.030 | -5.199 |
| 1-bromo-2,4,7,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.151 | -0.532 | 0.006 | -4.868 |
| 1-bromo-2,6,7,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.018 | -0.622 | 0.030 | -5.342 |
| 1-bromo-3,4,6,7,8-pentachlorodibenzo*-p-*dioxin | 2 | -3578.175 | 1.460 | -0.072 | -6.686 |
| 1-bromo-3,4,6,7,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.219 | 0.814 | -0.033 | -6.443 |
| 1-bromo-3,4,6,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.219 | 0.062 | 0.000 | -5.846 |
| 1-bromo-3,4,7,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.174 | 0.215 | -0.014 | -5.787 |
| 1-bromo-3,6,7,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.169 | 0.276 | -0.022 | -5.698 |
| 1-bromo-4,6,7,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.089 | 1.111 | -0.086 | -5.665 |
| 2-bromo-1,3,4,6,7-pentachlorodibenzo*-p-*dioxin | 2 | -3577.975 | 0.757 | -0.001 | -7.209 |
| 2-bromo-1,3,4,6,8-pentachlorodibenzo*-p-*dioxin | 2 | -3578.104 | -0.150 | 0.020 | -5.978 |
| 2-bromo-1,3,4,6,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.016 | -0.999 | 0.068 | -5.600 |
| 2-bromo-1,3,4,7,8-pentachlorodibenzo*-p-*dioxin | 2 | -3578.051 | 0.011 | 0.000 | -5.780 |
| 2-bromo-1,3,4,7,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.102 | -0.663 | 0.038 | -5.455 |
| 2-bromo-1,3,4,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3577.975 | -1.756 | 0.067 | -4.120 |
| 2-bromo-1,3,6,7,8-pentachlorodibenzo*-p-*dioxin | 2 | -3578.067 | 0.055 | -0.003 | -5.784 |
| 2-bromo-1,3,6,7,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.109 | -0.580 | 0.035 | -5.536 |
| 2-bromo-1,3,6,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.111 | -1.340 | 0.073 | -5.054 |
| 2-bromo-1,3,7,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.058 | -1.223 | 0.057 | -4.874 |
| 2-bromo-1,4,6,7,8-pentachlorodibenzo*-p-*dioxin | 2 | -3578.143 | 0.698 | -0.039 | -6.077 |
| 2-bromo-1,4,6,7,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.187 | 0.061 | -0.003 | -5.773 |
| 2-bromo-1,4,6,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.187 | -0.691 | 0.029 | -5.151 |
| 2-bromo-1,4,7,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.142 | -0.536 | 0.008 | -4.913 |
| 2-bromo-1,6,7,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.017 | -0.645 | 0.036 | -5.453 |
| 2-bromo-3,4,6,7,8-pentachlorodibenzo*-p-*dioxin | 2 | -3578.087 | 1.325 | -0.052 | -6.961 |
| 2-bromo-3,4,6,7,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.138 | 0.642 | -0.020 | -6.463 |
| 2-bromo-3,4,6,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.138 | -0.114 | 0.013 | -5.859 |
| 2-bromo-3,4,7,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.093 | 0.045 | -0.002 | -5.785 |
| 2-bromo-3,6,7,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.088 | 0.085 | -0.003 | -5.838 |
| 2-bromo-4,6,7,8,9-pentachlorodibenzo*-p-*dioxin | 2 | -3578.162 | 0.777 | -0.047 | -6.018 |
| 1,2-dibromo-3,4,6,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.499 | 0.784 | 0.001 | -12.292 |
| 1,2-dibromo-3,4,6,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.628 | -0.121 | 0.021 | -11.038 |
| 1,2-dibromo-3,4,6,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.539 | -0.968 | 0.063 | -10.509 |
| 1,2-dibromo-3,4,7,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.575 | 0.035 | 0.002 | -10.856 |
| 1,2-dibromo-3,4,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.626 | -0.637 | 0.038 | -10.483 |
| 1,2-dibromo-3,4,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.498 | -1.729 | 0.063 | -9.047 |
| 1,2-dibromo-3,6,7,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.588 | 0.093 | -0.003 | -10.836 |
| 1,2-dibromo-3,6,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.630 | -0.539 | 0.036 | -10.620 |
| 1,2-dibromo-3,6,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.631 | -1.298 | 0.068 | -9.984 |
| 1,2-dibromo-3,7,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.579 | -1.188 | 0.054 | -9.843 |
| 1,2-dibromo-4,6,7,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.669 | 0.731 | -0.038 | -11.145 |
| 1,2-dibromo-4,6,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.714 | 0.097 | -0.004 | -10.794 |
| 1,2-dibromo-4,6,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.712 | -0.655 | 0.026 | -10.121 |
| 1,2-dibromo-4,7,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.669 | -0.505 | 0.003 | -9.821 |
| 1,2-dibromo-6,7,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.540 | -0.607 | 0.033 | -10.427 |
| 1,3-dibromo-2,4,6,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.373 | 0.768 | 0.007 | -12.440 |
| 1,3-dibromo-2,4,6,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.499 | -0.140 | 0.021 | -11.026 |
| 1,3-dibromo-2,4,6,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.414 | -0.988 | 0.070 | -10.676 |
| 1,3-dibromo-2,4,7,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.449 | 0.018 | 0.002 | -10.847 |
| 1,3-dibromo-2,4,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.503 | -0.655 | 0.038 | -10.472 |
| 1,3-dibromo-2,6,7,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.491 | 0.073 | -0.003 | -10.816 |
| 1,3-dibromo-2,6,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.536 | -0.561 | 0.037 | -10.621 |
| 1,3-dibromo-2,6,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.535 | -1.317 | 0.070 | -10.017 |
| 1,3-dibromo-2,7,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.485 | -1.209 | 0.054 | -9.820 |
| 1,3-dibromo-4,6,7,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.584 | 1.448 | -0.075 | -11.585 |
| 1,3-dibromo-4,6,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.629 | 0.805 | -0.033 | -11.425 |
| 1,3-dibromo-4,6,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.628 | 0.056 | 0.005 | -10.965 |
| 1,3-dibromo-4,7,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.585 | 0.209 | -0.016 | -10.723 |
| 1,3-dibromo-6,7,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.600 | 0.266 | -0.021 | -10.701 |
| 1,4-dibromo-2,3,6,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.418 | 0.697 | 0.012 | -12.425 |
| 1,4-dibromo-2,3,6,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.547 | -0.218 | 0.027 | -11.022 |
| 1,4-dibromo-2,3,6,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.459 | -1.068 | 0.076 | -10.669 |
| 1,4-dibromo-2,3,7,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.495 | -0.051 | 0.005 | -10.783 |
| 1,4-dibromo-2,6,7,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.584 | 0.622 | -0.037 | -10.976 |
| 1,4-dibromo-2,6,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.629 | -0.014 | 0.001 | -10.725 |
| 1,4-dibromo-2,6,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.628 | -0.771 | 0.030 | -10.016 |
| 1,4-dibromo-2,7,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.585 | -0.615 | 0.002 | -9.599 |
| 1,4-dibromo-6,7,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.528 | 1.037 | -0.085 | -10.542 |
| 1,6-dibromo-2,3,4,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.428 | 0.705 | 0.007 | -12.308 |
| 1,6-dibromo-2,3,4,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.578 | -0.196 | 0.024 | -10.981 |
| 1,6-dibromo-2,3,4,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.499 | -1.030 | 0.076 | -10.734 |
| 1,6-dibromo-2,3,7,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.507 | 0.000 | 0.000 | -10.750 |
| 1,6-dibromo-2,3,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.558 | -0.615 | 0.041 | -10.616 |
| 1,6-dibromo-2,3,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.582 | -1.365 | 0.079 | -10.149 |
| 1,6-dibromo-2,4,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.611 | 0.000 | 0.005 | -10.860 |
| 1,6-dibromo-2,4,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.633 | -0.741 | 0.037 | -10.255 |
| 1,6-dibromo-3,4,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.658 | 0.001 | 0.010 | -10.983 |
| 1,7-dibromo-2,3,4,6-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.426 | 0.728 | 0.003 | -12.249 |
| 1,7-dibromo-2,3,4,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.497 | -0.009 | 0.002 | -10.786 |
| 1,7-dibromo-2,3,4,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.571 | -0.699 | 0.044 | -10.530 |
| 1,7-dibromo-2,3,6,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.473 | 0.039 | -0.001 | -10.805 |
| 1,7-dibromo-2,3,6,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.550 | -0.602 | 0.039 | -10.591 |
| 1,7-dibromo-2,3,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.494 | -1.235 | 0.059 | -9.898 |
| 1,7-dibromo-2,4,6,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.523 | 0.654 | -0.039 | -10.998 |
| 1,7-dibromo-2,4,6,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.601 | 0.015 | 0.001 | -10.787 |
| 1,7-dibromo-2,4,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.551 | -0.573 | 0.009 | -9.868 |
| 1,7-dibromo-2,6,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.387 | -0.675 | 0.034 | -10.351 |
| 1,7-dibromo-3,4,6,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.549 | 1.403 | -0.071 | -11.609 |
| 1,7-dibromo-3,4,6,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.626 | 0.755 | -0.032 | -11.355 |
| 1,7-dibromo-3,4,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.576 | 0.172 | -0.022 | -10.498 |
| 1,7-dibromo-3,6,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.539 | 0.221 | -0.021 | -10.625 |
| 1,7-dibromo-4,6,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.458 | 1.052 | -0.086 | -10.558 |
| 1,8-dibromo-2,3,4,6-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.571 | -0.112 | 0.020 | -11.041 |
| 1,8-dibromo-2,3,4,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.497 | 0.054 | 0.002 | -10.908 |
| 1,8-dibromo-2,3,4,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.426 | -1.729 | 0.073 | -9.320 |
| 1,8-dibromo-2,3,6,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.500 | 0.115 | -0.005 | -10.843 |
| 1,8-dibromo-2,3,6,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.549 | -1.285 | 0.070 | -10.077 |
| 1,8-dibromo-2,3,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.466 | -1.168 | 0.055 | -9.929 |
| 1,8-dibromo-2,4,6,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.552 | 0.732 | -0.039 | -11.143 |
| 1,8-dibromo-2,4,6,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.601 | -0.661 | 0.038 | -10.442 |
| 1,8-dibromo-2,4,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.526 | -0.507 | 0.007 | -9.948 |
| 1,8-dibromo-2,6,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.388 | -0.600 | 0.037 | -10.574 |
| 1,8-dibromo-3,4,6,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.577 | 1.474 | -0.074 | -11.663 |
| 1,8-dibromo-3,4,6,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.626 | 0.077 | 0.007 | -11.058 |
| 1,8-dibromo-3,4,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.548 | 0.235 | -0.016 | -10.780 |
| 1,8-dibromo-3,6,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.537 | 0.293 | -0.024 | -10.687 |
| 1,8-dibromo-4,6,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.459 | 1.127 | -0.074 | -11.015 |
| 1,9-dibromo-2,3,4,6-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.499 | -0.918 | 0.064 | -10.639 |
| 1,9-dibromo-2,3,4,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.580 | -0.559 | 0.034 | -10.539 |
| 1,9-dibromo-2,3,4,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.428 | -1.657 | 0.070 | -9.381 |
| 1,9-dibromo-2,3,6,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.582 | -0.470 | 0.031 | -10.632 |
| 1,9-dibromo-2,3,6,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.558 | -1.237 | 0.070 | -10.168 |
| 1,9-dibromo-2,3,7,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.500 | -1.107 | 0.056 | -10.066 |
| 1,9-dibromo-2,4,6,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.635 | 0.149 | -0.009 | -10.780 |
| 1,9-dibromo-2,4,6,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.608 | -0.609 | 0.029 | -10.307 |
| 1,9-dibromo-3,4,6,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.658 | 0.891 | -0.042 | -11.352 |
| 2,3-dibromo-1,4,6,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.464 | 0.726 | -0.001 | -12.134 |
| 2,3-dibromo-1,4,6,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.592 | -0.179 | 0.020 | -10.907 |
| 2,3-dibromo-1,4,6,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.505 | -1.025 | 0.065 | -10.457 |
| 2,3-dibromo-1,4,7,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.540 | -0.015 | 0.001 | -10.740 |
| 2,3-dibromo-1,6,7,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.587 | 0.026 | -0.001 | -10.759 |
| 2,3-dibromo-1,6,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.631 | -0.608 | 0.037 | -10.512 |
| 2,3-dibromo-1,6,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.632 | -1.363 | 0.073 | -9.988 |
| 2,3-dibromo-1,7,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.580 | -1.247 | 0.057 | -9.807 |
| 2,3-dibromo-6,7,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.611 | 0.063 | -0.003 | -10.774 |
| 2,7-dibromo-1,3,4,6-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.386 | 0.702 | 0.001 | -12.155 |
| 2,7-dibromo-1,3,4,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.458 | -0.027 | 0.002 | -10.759 |
| 2,7-dibromo-1,3,4,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.530 | -0.716 | 0.042 | -10.452 |
| 2,7-dibromo-1,3,6,8-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.442 | 0.000 | 0.001 | -10.788 |
| 2,7-dibromo-1,3,6,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.517 | -0.639 | 0.040 | -10.552 |
| 2,7-dibromo-1,3,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.462 | -1.264 | 0.063 | -9.952 |
| 2,7-dibromo-1,4,6,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.594 | 0.000 | 0.002 | -10.785 |
| 2,7-dibromo-1,4,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.544 | -0.579 | 0.013 | -9.961 |
| 2,7-dibromo-3,4,8,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.495 | 0.000 | 0.001 | -10.778 |
| 2,8-dibromo-1,3,4,6-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.532 | -0.135 | 0.018 | -10.952 |
| 2,8-dibromo-1,3,4,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.456 | 0.036 | 0.000 | -10.829 |
| 2,8-dibromo-1,3,4,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.385 | -1.742 | 0.068 | -9.172 |
| 2,8-dibromo-1,3,6,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.467 | 0.077 | -0.003 | -10.828 |
| 2,8-dibromo-1,3,6,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.516 | -1.320 | 0.073 | -10.093 |
| 2,8-dibromo-1,3,7,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.431 | -1.197 | 0.056 | -9.905 |
| 2,8-dibromo-1,4,6,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.545 | 0.718 | -0.039 | -11.117 |
| 2,8-dibromo-1,4,6,9-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.594 | -0.673 | 0.033 | -10.290 |
| 2,8-dibromo-3,4,6,7-tetrachlorodibenzo*-p-*dioxin | 2 | -3551.489 | 1.340 | -0.055 | -11.914 |
| 1,2,3-tribromo-4,6,7-trichlorodibenzo*-p-*dioxin | 2 | -3524.991 | 0.766 | 0.012 | -17.527 |
| 1,2,3-tribromo-4,6,8-trichlorodibenzo*-p-*dioxin | 2 | -3525.118 | -0.137 | 0.019 | -15.940 |
| 1,2,3-tribromo-4,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.031 | -0.982 | 0.066 | -15.545 |
| 1,2,3-tribromo-4,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3525.066 | 0.022 | 0.002 | -15.816 |
| 1,2,3-tribromo-4,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.119 | -0.648 | 0.038 | -15.446 |
| 1,2,3-tribromo-4,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.990 | -1.737 | 0.063 | -14.016 |
| 1,2,3-tribromo-6,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3525.110 | 0.073 | -0.003 | -15.776 |
| 1,2,3-tribromo-6,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.154 | -0.558 | 0.035 | -15.536 |
| 1,2,3-tribromo-6,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.154 | -1.312 | 0.068 | -14.936 |
| 1,2,3-tribromo-7,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.103 | -1.202 | 0.051 | -14.716 |
| 1,2,4-tribromo-3,6,7-trichlorodibenzo*-p-*dioxin | 2 | -3524.893 | 0.697 | 0.014 | -17.464 |
| 1,2,4-tribromo-3,6,8-trichlorodibenzo*-p-*dioxin | 2 | -3525.023 | -0.213 | 0.025 | -15.967 |
| 1,2,4-tribromo-3,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.934 | -1.062 | 0.069 | -15.486 |
| 1,2,4-tribromo-3,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.969 | -0.046 | 0.004 | -15.755 |
| 1,2,4-tribromo-3,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.020 | -0.718 | 0.039 | -15.356 |
| 1,2,4-tribromo-3,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.893 | -1.816 | 0.068 | -14.011 |
| 1,2,4-tribromo-6,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3525.107 | 0.641 | -0.037 | -15.992 |
| 1,2,4-tribromo-6,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.151 | 0.006 | 0.002 | -15.769 |
| 1,2,4-tribromo-6,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.150 | -0.749 | 0.026 | -14.934 |
| 1,2,4-tribromo-7,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.106 | -0.590 | 0.001 | -14.600 |
| 1,2,6-tribromo-3,4,7-trichlorodibenzo*-p-*dioxin | 2 | -3524.912 | 0.703 | 0.000 | -17.109 |
| 1,2,6-tribromo-3,4,8-trichlorodibenzo*-p-*dioxin | 2 | -3525.063 | -0.191 | 0.025 | -16.002 |
| 1,2,6-tribromo-3,4,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.983 | -1.023 | 0.068 | -15.526 |
| 1,2,6-tribromo-3,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.995 | -0.001 | 0.001 | -15.759 |
| 1,2,6-tribromo-3,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.045 | -0.613 | 0.037 | -15.502 |
| 1,2,6-tribromo-3,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.070 | -1.360 | 0.075 | -15.040 |
| 1,2,6-tribromo-4,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3525.077 | 0.634 | -0.038 | -15.958 |
| 1,2,6-tribromo-4,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.129 | 0.020 | -0.001 | -15.722 |
| 1,2,6-tribromo-4,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.152 | -0.718 | 0.033 | -15.175 |
| 1,2,6-tribromo-7,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.950 | -0.688 | 0.042 | -15.505 |
| 1,2,7-tribromo-3,4,6-trichlorodibenzo*-p-*dioxin | 2 | -3524.911 | 0.731 | 0.005 | -17.293 |
| 1,2,7-tribromo-3,4,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.981 | -0.001 | 0.004 | -15.839 |
| 1,2,7-tribromo-3,4,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.054 | -0.689 | 0.040 | -15.431 |
| 1,2,7-tribromo-3,6,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.963 | 0.040 | -0.002 | -15.766 |
| 1,2,7-tribromo-3,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.038 | -0.597 | 0.037 | -15.534 |
| 1,2,7-tribromo-3,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.982 | -1.227 | 0.057 | -14.847 |
| 1,2,7-tribromo-4,6,8-trichlorodibenzo*-p-*dioxin | 2 | -3525.043 | 0.675 | -0.039 | -16.017 |
| 1,2,7-tribromo-4,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.120 | 0.037 | 0.000 | -15.783 |
| 1,2,7-tribromo-4,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.070 | -0.547 | 0.007 | -14.846 |
| 1,2,7-tribromo-6,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.909 | -0.660 | 0.033 | -15.333 |
| 1,2,8-tribromo-3,4,6-trichlorodibenzo*-p-*dioxin | 2 | -3525.056 | -0.105 | 0.019 | -16.014 |
| 1,2,8-tribromo-3,4,7-trichlorodibenzo*-p-*dioxin | 2 | -3524.981 | 0.061 | 0.001 | -15.881 |
| 1,2,8-tribromo-3,4,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.909 | -1.715 | 0.068 | -14.203 |
| 1,2,8-tribromo-3,6,7-trichlorodibenzo*-p-*dioxin | 2 | -3524.989 | 0.116 | -0.003 | -15.882 |
| 1,2,8-tribromo-3,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.037 | -1.278 | 0.068 | -15.023 |
| 1,2,8-tribromo-3,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.953 | -1.160 | 0.052 | -14.852 |
| 1,2,8-tribromo-4,6,7-trichlorodibenzo*-p-*dioxin | 2 | -3525.071 | 0.752 | -0.038 | -16.187 |
| 1,2,8-tribromo-4,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.120 | -0.636 | 0.027 | -15.184 |
| 1,2,8-tribromo-4,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.043 | -0.480 | 0.007 | -14.980 |
| 1,2,8-tribromo-6,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.909 | -0.585 | 0.032 | -15.452 |
| 1,2,9-tribromo-3,4,6-trichlorodibenzo*-p-*dioxin | 2 | -3524.983 | -0.906 | 0.057 | -15.467 |
| 1,2,9-tribromo-3,4,7-trichlorodibenzo*-p-*dioxin | 2 | -3525.062 | -0.547 | 0.032 | -15.496 |
| 1,2,9-tribromo-3,4,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.912 | -1.640 | 0.067 | -14.322 |
| 1,2,9-tribromo-3,6,7-trichlorodibenzo*-p-*dioxin | 2 | -3525.070 | -0.464 | 0.030 | -15.603 |
| 1,2,9-tribromo-3,6,8-trichlorodibenzo*-p-*dioxin | 2 | -3525.047 | -1.228 | 0.066 | -15.066 |
| 1,2,9-tribromo-3,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.988 | -1.097 | 0.054 | -15.019 |
| 1,2,9-tribromo-4,6,7-trichlorodibenzo*-p-*dioxin | 2 | -3525.153 | 0.173 | -0.006 | -15.884 |
| 1,2,9-tribromo-4,6,8-trichlorodibenzo*-p-*dioxin | 2 | -3525.127 | -0.583 | 0.025 | -15.233 |
| 1,2,9-tribromo-4,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3525.076 | -0.413 | 0.008 | -15.129 |
| 1,2,9-tribromo-6,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.950 | -0.532 | 0.033 | -15.572 |
| 1,3,6-tribromo-2,4,7-trichlorodibenzo*-p-*dioxin | 2 | -3524.787 | 0.688 | 0.004 | -17.207 |
| 1,3,6-tribromo-2,4,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.936 | -0.208 | 0.023 | -15.941 |
| 1,3,6-tribromo-2,4,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.858 | -1.041 | 0.075 | -15.697 |
| 1,3,6-tribromo-2,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.899 | -0.021 | 0.001 | -15.738 |
| 1,3,6-tribromo-2,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.952 | -0.634 | 0.041 | -15.583 |
| 1,3,6-tribromo-2,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.975 | -1.378 | 0.078 | -15.102 |
| 1,3,6-tribromo-4,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.992 | 1.353 | -0.073 | -16.454 |
| 1,3,6-tribromo-4,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.044 | 0.731 | -0.027 | -16.437 |
| 1,3,6-tribromo-4,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.068 | -0.006 | 0.009 | -15.943 |
| 1,3,6-tribromo-7,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.010 | 0.185 | -0.019 | -15.596 |
| 1,3,7-tribromo-2,4,6-trichlorodibenzo*-p-*dioxin | 2 | -3524.784 | 0.713 | 0.005 | -17.282 |
| 1,3,7-tribromo-2,4,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.854 | -0.019 | 0.002 | -15.777 |
| 1,3,7-tribromo-2,4,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.930 | -0.708 | 0.042 | -15.470 |
| 1,3,7-tribromo-2,6,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.865 | 0.020 | -0.001 | -15.772 |
| 1,3,7-tribromo-2,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.942 | -0.619 | 0.043 | -15.665 |
| 1,3,7-tribromo-2,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.887 | -1.247 | 0.059 | -14.878 |
| 1,3,7-tribromo-4,6,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.958 | 1.391 | -0.071 | -16.586 |
| 1,3,7-tribromo-4,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.035 | 0.745 | -0.029 | -16.414 |
| 1,3,7-tribromo-4,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.986 | 0.166 | -0.020 | -15.538 |
| 1,3,7-tribromo-6,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.970 | 0.210 | -0.019 | -15.652 |
| 1,3,8-tribromo-2,4,6-trichlorodibenzo*-p-*dioxin | 2 | -3524.928 | -0.122 | 0.030 | -16.291 |
| 1,3,8-tribromo-2,4,7-trichlorodibenzo*-p-*dioxin | 2 | -3524.856 | 0.045 | 0.000 | -15.848 |
| 1,3,8-tribromo-2,4,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.785 | -1.732 | 0.071 | -14.272 |
| 1,3,8-tribromo-2,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.942 | -1.297 | 0.070 | -15.057 |
| 1,3,8-tribromo-2,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.860 | -1.182 | 0.053 | -14.853 |
| 1,3,8-tribromo-4,6,7-trichlorodibenzo*-p-*dioxin | 2 | -3524.986 | 1.464 | -0.064 | -16.903 |
| 1,3,8-tribromo-4,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.035 | 0.071 | 0.006 | -16.020 |
| 1,3,8-tribromo-4,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.959 | 0.230 | -0.017 | -15.745 |
| 1,3,8-tribromo-6,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.969 | 0.282 | -0.023 | -15.687 |
| 1,3,9-tribromo-2,4,6-trichlorodibenzo*-p-*dioxin | 2 | -3524.857 | -0.929 | 0.064 | -15.628 |
| 1,3,9-tribromo-2,4,7-trichlorodibenzo*-p-*dioxin | 2 | -3524.939 | -0.568 | 0.035 | -15.557 |
| 1,3,9-tribromo-2,4,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.786 | -1.661 | 0.071 | -14.409 |
| 1,3,9-tribromo-2,6,7-trichlorodibenzo*-p-*dioxin | 2 | -3524.975 | -0.488 | 0.032 | -15.627 |
| 1,3,9-tribromo-2,6,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.950 | -1.250 | 0.070 | -15.146 |
| 1,3,9-tribromo-2,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.893 | -1.122 | 0.055 | -15.014 |
| 1,3,9-tribromo-4,6,7-trichlorodibenzo*-p-*dioxin | 2 | -3525.068 | 0.881 | -0.042 | -16.333 |
| 1,3,9-tribromo-4,6,8-trichlorodibenzo*-p-*dioxin | 2 | -3525.043 | 0.128 | -0.004 | -15.869 |
| 1,3,9-tribromo-4,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.992 | 0.302 | -0.018 | -15.851 |
| 1,3,9-tribromo-6,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3525.010 | 0.340 | -0.026 | -15.714 |
| 1,4,6-tribromo-2,3,7-trichlorodibenzo*-p-*dioxin | 2 | -3524.833 | 0.631 | 0.018 | -17.452 |
| 1,4,6-tribromo-2,3,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.984 | -0.273 | 0.028 | -15.937 |
| 1,4,6-tribromo-2,3,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.904 | -1.108 | 0.079 | -15.663 |
| 1,4,6-tribromo-2,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.993 | 0.539 | -0.035 | -15.868 |
| 1,4,6-tribromo-2,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.046 | -0.077 | 0.006 | -15.732 |
| 1,4,6-tribromo-2,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.069 | -0.821 | 0.035 | -15.044 |
| 1,4,6-tribromo-3,7,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.994 | 1.297 | -0.068 | -16.475 |
| 1,4,6-tribromo-3,7,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.044 | 0.671 | -0.029 | -16.269 |
| 1,4,6-tribromo-3,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.069 | -0.074 | 0.015 | -15.967 |
| 1,4,6-tribromo-7,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.939 | 0.966 | -0.082 | -15.483 |
| 1,4,7-tribromo-2,3,6-trichlorodibenzo*-p-*dioxin | 2 | -3524.830 | 0.641 | 0.015 | -17.394 |
| 1,4,7-tribromo-2,3,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.901 | -0.089 | 0.006 | -15.736 |
| 1,4,7-tribromo-2,3,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.975 | -0.780 | 0.045 | -15.400 |
| 1,4,7-tribromo-2,6,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.958 | 0.564 | -0.034 | -15.949 |
| 1,4,7-tribromo-2,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.036 | -0.075 | 0.005 | -15.712 |
| 1,4,7-tribromo-2,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.986 | -0.657 | 0.005 | -14.597 |
| 1,4,7-tribromo-3,6,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.960 | 1.320 | -0.064 | -16.630 |
| 1,4,7-tribromo-3,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.035 | 0.671 | -0.024 | -16.401 |
| 1,4,7-tribromo-3,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.986 | 0.095 | -0.018 | -15.453 |
| 1,4,7-tribromo-6,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.897 | 0.976 | -0.087 | -15.380 |
| 1,7,8-tribromo-2,3,4-trichlorodibenzo*-p-*dioxin | 2 | -3525.020 | 0.014 | 0.004 | -15.861 |
| 1,7,8-tribromo-2,3,6-trichlorodibenzo*-p-*dioxin | 2 | -3524.994 | 0.068 | -0.002 | -15.814 |
| 1,7,8-tribromo-2,3,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.987 | -1.208 | 0.059 | -14.934 |
| 1,7,8-tribromo-2,4,6-trichlorodibenzo*-p-*dioxin | 2 | -3525.045 | 0.682 | -0.039 | -16.030 |
| 1,7,8-tribromo-2,4,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.046 | -0.549 | 0.007 | -14.846 |
| 1,7,8-tribromo-2,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.877 | -0.643 | 0.033 | -15.372 |
| 1,7,8-tribromo-3,4,6-trichlorodibenzo*-p-*dioxin | 2 | -3525.070 | 1.426 | -0.072 | -16.606 |
| 1,7,8-tribromo-3,4,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.070 | 0.193 | -0.019 | -15.600 |
| 1,7,8-tribromo-3,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.028 | 0.249 | -0.021 | -15.665 |
| 1,7,8-tribromo-4,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.948 | 1.079 | -0.081 | -15.725 |
| 2,3,7-tribromo-1,4,6-trichlorodibenzo*-p-*dioxin | 2 | -3524.875 | 0.670 | 0.002 | -17.104 |
| 2,3,7-tribromo-1,4,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.946 | -0.053 | 0.002 | -15.694 |
| 2,3,7-tribromo-1,4,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.020 | -0.740 | 0.043 | -15.417 |
| 2,3,7-tribromo-1,6,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.962 | -0.029 | 0.002 | -15.737 |
| 2,3,7-tribromo-1,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.038 | -0.667 | 0.042 | -15.529 |
| 2,3,7-tribromo-1,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.983 | -1.287 | 0.064 | -14.912 |
| 2,3,7-tribromo-4,6,8-trichlorodibenzo*-p-*dioxin | 2 | -3524.954 | 1.238 | -0.053 | -16.758 |
| 2,3,7-tribromo-4,6,9-trichlorodibenzo*-p-*dioxin | 2 | -3525.038 | 0.555 | -0.016 | -16.384 |
| 2,3,7-tribromo-4,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.989 | -0.019 | 0.002 | -15.751 |
| 2,3,7-tribromo-6,8,9-trichlorodibenzo*-p-*dioxin | 2 | -3524.980 | 0.005 | 0.000 | -15.747 |
| 1,2,3,4-tetrabromo-6,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.513 | 0.681 | 0.012 | -22.342 |
| 1,2,3,4-tetrabromo-6,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.641 | -0.225 | 0.026 | -20.931 |
| 1,2,3,4-tetrabromo-6,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.553 | -1.069 | 0.069 | -20.433 |
| 1,2,3,4-tetrabromo-7,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.589 | -0.058 | 0.005 | -20.718 |
| 1,2,3,6-tetrabromo-4,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.405 | 0.685 | 0.008 | -22.266 |
| 1,2,3,6-tetrabromo-4,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.554 | -0.207 | 0.022 | -20.878 |
| 1,2,3,6-tetrabromo-4,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.475 | -1.038 | 0.069 | -20.508 |
| 1,2,3,6-tetrabromo-7,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.518 | -0.021 | 0.000 | -20.673 |
| 1,2,3,6-tetrabromo-7,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.569 | -0.633 | 0.039 | -20.494 |
| 1,2,3,6-tetrabromo-8,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.593 | -1.374 | 0.076 | -20.018 |
| 1,2,3,7-tetrabromo-4,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.402 | 0.711 | 0.004 | -22.213 |
| 1,2,3,7-tetrabromo-4,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.472 | -0.015 | 0.002 | -20.745 |
| 1,2,3,7-tetrabromo-4,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.547 | -0.701 | 0.041 | -20.418 |
| 1,2,3,7-tetrabromo-6,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.485 | 0.020 | -0.001 | -20.732 |
| 1,2,3,7-tetrabromo-6,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.561 | -0.616 | 0.039 | -20.528 |
| 1,2,3,7-tetrabromo-8,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.505 | -1.241 | 0.058 | -19.824 |
| 1,2,3,8-tetrabromo-4,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.546 | -0.121 | 0.020 | -20.994 |
| 1,2,3,8-tetrabromo-4,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.473 | 0.049 | 0.000 | -20.817 |
| 1,2,3,8-tetrabromo-4,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.401 | -1.723 | 0.071 | -19.250 |
| 1,2,3,8-tetrabromo-6,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.512 | 0.096 | -0.004 | -20.796 |
| 1,2,3,8-tetrabromo-6,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.560 | -1.292 | 0.067 | -19.949 |
| 1,2,3,8-tetrabromo-7,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.477 | -1.175 | 0.051 | -19.775 |
| 1,2,3,9-tetrabromo-4,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.475 | -0.921 | 0.059 | -20.474 |
| 1,2,3,9-tetrabromo-4,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.555 | -0.559 | 0.032 | -20.457 |
| 1,2,3,9-tetrabromo-4,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.403 | -1.649 | 0.066 | -19.263 |
| 1,2,3,9-tetrabromo-6,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.593 | -0.483 | 0.030 | -20.545 |
| 1,2,3,9-tetrabromo-6,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.569 | -1.243 | 0.067 | -20.042 |
| 1,2,3,9-tetrabromo-7,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.511 | -1.112 | 0.052 | -19.917 |
| 1,2,4,6-tetrabromo-3,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.308 | 0.628 | 0.010 | -22.226 |
| 1,2,4,6-tetrabromo-3,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.459 | -0.271 | 0.026 | -20.876 |
| 1,2,4,6-tetrabromo-3,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.378 | -1.103 | 0.075 | -20.556 |
| 1,2,4,6-tetrabromo-7,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.516 | 0.556 | -0.036 | -20.853 |
| 1,2,4,6-tetrabromo-7,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.567 | -0.058 | 0.003 | -20.670 |
| 1,2,4,6-tetrabromo-8,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.590 | -0.800 | 0.032 | -19.985 |
| 1,2,4,7-tetrabromo-3,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.305 | 0.641 | 0.018 | -22.459 |
| 1,2,4,7-tetrabromo-3,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.376 | -0.084 | 0.006 | -20.734 |
| 1,2,4,7-tetrabromo-3,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.449 | -0.772 | 0.043 | -20.352 |
| 1,2,4,7-tetrabromo-6,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.481 | 0.583 | -0.035 | -20.938 |
| 1,2,4,7-tetrabromo-6,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.557 | -0.054 | 0.004 | -20.706 |
| 1,2,4,7-tetrabromo-8,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.508 | -0.633 | 0.005 | -19.622 |
| 1,2,4,8-tetrabromo-3,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.450 | -0.196 | 0.025 | -20.997 |
| 1,2,4,8-tetrabromo-3,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.375 | -0.018 | 0.004 | -20.809 |
| 1,2,4,8-tetrabromo-3,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.304 | -1.800 | 0.061 | -18.860 |
| 1,2,4,8-tetrabromo-6,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.508 | 0.663 | -0.036 | -21.062 |
| 1,2,4,8-tetrabromo-6,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.557 | -0.729 | 0.029 | -20.051 |
| 1,2,4,8-tetrabromo-7,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.481 | -0.564 | 0.004 | -19.735 |
| 1,2,4,9-tetrabromo-3,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.379 | -0.999 | 0.064 | -20.471 |
| 1,2,4,9-tetrabromo-3,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.457 | -0.628 | 0.035 | -20.420 |
| 1,2,4,9-tetrabromo-3,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.308 | -1.727 | 0.063 | -19.052 |
| 1,2,4,9-tetrabromo-6,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.591 | 0.083 | 0.000 | -20.860 |
| 1,2,4,9-tetrabromo-6,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.566 | -0.677 | 0.026 | -20.072 |
| 1,2,4,9-tetrabromo-7,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.515 | -0.498 | 0.003 | -19.830 |
| 1,2,6,7-tetrabromo-3,4-dichlorodibenzo*-p-*dioxin | 2 | -3498.435 | 0.690 | 0.000 | -22.062 |
| 1,2,6,7-tetrabromo-3,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.484 | 0.000 | 0.001 | -20.746 |
| 1,2,6,7-tetrabromo-3,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.564 | -0.633 | 0.041 | -20.546 |
| 1,2,6,7-tetrabromo-4,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.647 | 0.000 | 0.001 | -20.715 |
| 1,2,6,8-tetrabromo-3,4-dichlorodibenzo*-p-*dioxin | 2 | -3498.495 | -0.180 | 0.021 | -20.915 |
| 1,2,6,8-tetrabromo-3,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.387 | 0.019 | -0.001 | -20.749 |
| 1,2,6,8-tetrabromo-3,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.479 | -1.348 | 0.076 | -20.090 |
| 1,2,6,8-tetrabromo-4,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.470 | 0.653 | -0.036 | -21.049 |
| 1,2,6,8-tetrabromo-4,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.562 | -0.707 | 0.037 | -20.300 |
| 1,2,6,8-tetrabromo-7,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.309 | -0.672 | 0.043 | -20.571 |
| 1,2,6,9-tetrabromo-3,4-dichlorodibenzo*-p-*dioxin | 2 | -3498.422 | -0.957 | 0.062 | -20.492 |
| 1,2,6,9-tetrabromo-3,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.481 | -0.535 | 0.032 | -20.518 |
| 1,2,6,9-tetrabromo-3,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.482 | -1.289 | 0.075 | -20.177 |
| 1,2,6,9-tetrabromo-4,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.564 | 0.100 | -0.003 | -20.820 |
| 1,2,6,9-tetrabromo-4,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.563 | -0.646 | 0.032 | -20.288 |
| 1,2,6,9-tetrabromo-7,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.355 | -0.613 | 0.040 | -20.598 |
| 1,2,7,8-tetrabromo-3,4-dichlorodibenzo*-p-*dioxin | 2 | -3498.504 | 0.021 | 0.003 | -20.835 |
| 1,2,7,8-tetrabromo-3,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.483 | 0.069 | -0.003 | -20.775 |
| 1,2,7,8-tetrabromo-3,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.475 | -1.200 | 0.057 | -19.883 |
| 1,2,7,8-tetrabromo-4,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.564 | 0.703 | -0.040 | -21.024 |
| 1,2,7,8-tetrabromo-4,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.564 | -0.522 | 0.008 | -19.904 |
| 1,2,7,8-tetrabromo-6,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.399 | -0.628 | 0.035 | -20.431 |
| 1,2,7,9-tetrabromo-3,4-dichlorodibenzo*-p-*dioxin | 2 | -3498.494 | -0.598 | 0.037 | -20.523 |
| 1,2,7,9-tetrabromo-3,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.481 | -0.522 | 0.032 | -20.543 |
| 1,2,7,9-tetrabromo-3,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.381 | -1.133 | 0.059 | -20.082 |
| 1,2,7,9-tetrabromo-4,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.562 | 0.112 | -0.004 | -20.818 |
| 1,2,7,9-tetrabromo-4,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.468 | -0.452 | 0.010 | -20.109 |
| 1,2,7,9-tetrabromo-6,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.309 | -0.586 | 0.035 | -20.529 |
| 1,2,8,9-tetrabromo-3,4-dichlorodibenzo*-p-*dioxin | 2 | -3498.434 | -1.630 | 0.066 | -19.294 |
| 1,2,8,9-tetrabromo-3,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.564 | -1.212 | 0.066 | -20.077 |
| 1,2,8,9-tetrabromo-3,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.475 | -1.071 | 0.053 | -20.029 |
| 1,2,8,9-tetrabromo-4,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.646 | -0.570 | 0.025 | -20.237 |
| 1,3,6,8-tetrabromo-2,4-dichlorodibenzo*-p-*dioxin | 2 | -3498.369 | -0.196 | 0.023 | -20.960 |
| 1,3,6,8-tetrabromo-2,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.292 | 0.000 | 0.002 | -20.808 |
| 1,3,6,8-tetrabromo-2,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.385 | -1.366 | 0.088 | -20.384 |
| 1,3,6,8-tetrabromo-4,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.478 | 0.001 | 0.009 | -20.957 |
| 1,3,6,9-tetrabromo-2,4-dichlorodibenzo*-p-*dioxin | 2 | -3498.297 | -0.978 | 0.070 | -20.683 |
| 1,3,6,9-tetrabromo-2,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.387 | -0.559 | 0.037 | -20.619 |
| 1,3,6,9-tetrabromo-2,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.386 | -1.310 | 0.077 | -20.207 |
| 1,3,6,9-tetrabromo-4,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.479 | 0.810 | -0.035 | -21.377 |
| 1,3,6,9-tetrabromo-4,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.479 | 0.066 | 0.003 | -20.926 |
| 1,3,6,9-tetrabromo-7,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.415 | 0.260 | -0.020 | -20.716 |
| 1,3,7,8-tetrabromo-2,4-dichlorodibenzo*-p-*dioxin | 2 | -3498.379 | 0.004 | 0.001 | -20.773 |
| 1,3,7,8-tetrabromo-2,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.386 | 0.049 | -0.002 | -20.781 |
| 1,3,7,8-tetrabromo-2,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.381 | -1.221 | 0.058 | -19.886 |
| 1,3,7,8-tetrabromo-4,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.479 | 1.414 | -0.073 | -21.557 |
| 1,3,7,8-tetrabromo-4,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.480 | 0.187 | -0.012 | -20.770 |
| 1,3,7,8-tetrabromo-6,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.459 | 0.238 | -0.021 | -20.639 |
| 1,3,7,9-tetrabromo-2,4-dichlorodibenzo*-p-*dioxin | 2 | -3498.369 | -0.619 | 0.041 | -20.610 |
| 1,3,7,9-tetrabromo-2,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.385 | -0.547 | 0.036 | -20.617 |
| 1,3,7,9-tetrabromo-2,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.286 | -1.157 | 0.060 | -20.080 |
| 1,4,6,9-tetrabromo-2,3-dichlorodibenzo*-p-*dioxin | 2 | -3498.344 | -1.045 | 0.076 | -20.701 |
| 1,4,6,9-tetrabromo-2,7-dichlorodibenzo*-p-*dioxin | 2 | -3498.482 | 0.000 | 0.000 | -20.720 |
| 1,4,6,9-tetrabromo-2,8-dichlorodibenzo*-p-*dioxin | 2 | -3498.480 | -0.751 | 0.036 | -20.204 |
| 1,4,7,8-tetrabromo-2,3-dichlorodibenzo*-p-*dioxin | 2 | -3498.424 | -0.065 | 0.006 | -20.761 |
| 1,4,7,8-tetrabromo-2,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.480 | 0.594 | -0.036 | -20.934 |
| 1,4,7,8-tetrabromo-2,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.481 | -0.632 | 0.008 | -19.707 |
| 1,4,7,8-tetrabromo-6,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.387 | 1.004 | -0.083 | -20.523 |
| 2,3,7,8-tetrabromo-1,4-dichlorodibenzo*-p-*dioxin | 2 | -3498.469 | -0.031 | 0.002 | -20.715 |
| 2,3,7,8-tetrabromo-1,6-dichlorodibenzo*-p-*dioxin | 2 | -3498.483 | 0.000 | 0.001 | -20.746 |
| 2,3,7,8-tetrabromo-1,9-dichlorodibenzo*-p-*dioxin | 2 | -3498.476 | -1.261 | 0.064 | -19.947 |
| 1,2,3,4,6-pentabromo-7-chlorodibenzo*-p-*dioxin | 2 | -3471.927 | 0.610 | 0.009 | -27.126 |
| 1,2,3,4,6-pentabromo-8-chlorodibenzo*-p-*dioxin | 2 | -3472.077 | -0.283 | 0.027 | -25.840 |
| 1,2,3,4,6-pentabromo-9-chlorodibenzo*-p-*dioxin | 2 | -3471.997 | -1.113 | 0.077 | -25.549 |
| 1,2,3,4,7-pentabromo-6-chlorodibenzo*-p-*dioxin | 2 | -3471.924 | 0.625 | 0.015 | -27.311 |
| 1,2,3,4,7-pentabromo-8-chlorodibenzo*-p-*dioxin | 2 | -3471.995 | -0.096 | 0.004 | -25.619 |
| 1,2,3,4,7-pentabromo-9-chlorodibenzo*-p-*dioxin | 2 | -3472.069 | -0.781 | 0.046 | -25.372 |
| 1,2,3,6,7-pentabromo-4-chlorodibenzo*-p-*dioxin | 2 | -3471.926 | 0.670 | 0.001 | -27.034 |
| 1,2,3,6,7-pentabromo-8-chlorodibenzo*-p-*dioxin | 2 | -3472.006 | -0.020 | 0.001 | -25.686 |
| 1,2,3,6,7-pentabromo-9-chlorodibenzo*-p-*dioxin | 2 | -3472.088 | -0.652 | 0.042 | -25.514 |
| 1,2,3,6,8-pentabromo-4-chlorodibenzo*-p-*dioxin | 2 | -3471.986 | -0.196 | 0.020 | -25.843 |
| 1,2,3,6,8-pentabromo-7-chlorodibenzo*-p-*dioxin | 2 | -3471.911 | -0.002 | 0.000 | -25.713 |
| 1,2,3,6,8-pentabromo-9-chlorodibenzo*-p-*dioxin | 2 | -3472.003 | -1.362 | 0.076 | -25.041 |
| 1,2,3,6,9-pentabromo-4-chlorodibenzo*-p-*dioxin | 2 | -3471.915 | -0.973 | 0.066 | -25.550 |
| 1,2,3,6,9-pentabromo-7-chlorodibenzo*-p-*dioxin | 2 | -3472.004 | -0.555 | 0.034 | -25.510 |
| 1,2,3,6,9-pentabromo-8-chlorodibenzo*-p-*dioxin | 2 | -3472.005 | -1.305 | 0.074 | -25.099 |
| 1,2,3,7,8-pentabromo-4-chlorodibenzo*-p-*dioxin | 2 | -3471.996 | 0.008 | 0.002 | -25.768 |
| 1,2,3,7,8-pentabromo-6-chlorodibenzo*-p-*dioxin | 2 | -3472.006 | 0.049 | -0.002 | -25.742 |
| 1,2,3,7,8-pentabromo-9-chlorodibenzo*-p-*dioxin | 2 | -3471.999 | -1.214 | 0.055 | -24.783 |
| 1,2,3,7,9-pentabromo-4-chlorodibenzo*-p-*dioxin | 2 | -3471.986 | -0.611 | 0.035 | -25.431 |
| 1,2,3,7,9-pentabromo-6-chlorodibenzo*-p-*dioxin | 2 | -3472.003 | -0.543 | 0.033 | -25.507 |
| 1,2,3,7,9-pentabromo-8-chlorodibenzo*-p-*dioxin | 2 | -3471.904 | -1.148 | 0.061 | -25.084 |
| 1,2,3,8,9-pentabromo-4-chlorodibenzo*-p-*dioxin | 2 | -3471.926 | -1.638 | 0.072 | -24.419 |
| 1,2,3,8,9-pentabromo-6-chlorodibenzo*-p-*dioxin | 2 | -3472.087 | -1.227 | 0.066 | -25.027 |
| 1,2,3,8,9-pentabromo-7-chlorodibenzo*-p-*dioxin | 2 | -3471.999 | -1.087 | 0.052 | -24.950 |
| 1,2,4,6,7-pentabromo-3-chlorodibenzo*-p-*dioxin | 2 | -3471.830 | 0.613 | 0.013 | -27.254 |
| 1,2,4,6,7-pentabromo-8-chlorodibenzo*-p-*dioxin | 2 | -3472.003 | 0.552 | -0.034 | -25.883 |
| 1,2,4,6,7-pentabromo-9-chlorodibenzo*-p-*dioxin | 2 | -3472.085 | -0.081 | 0.006 | -25.683 |
| 1,2,4,6,8-pentabromo-3-chlorodibenzo*-p-*dioxin | 2 | -3471.890 | -0.258 | 0.027 | -25.923 |
| 1,2,4,6,8-pentabromo-7-chlorodibenzo*-p-*dioxin | 2 | -3471.908 | 0.576 | -0.034 | -25.947 |
| 1,2,4,6,8-pentabromo-9-chlorodibenzo*-p-*dioxin | 2 | -3472.000 | -0.789 | 0.037 | -25.136 |
| 1,2,4,6,9-pentabromo-3-chlorodibenzo*-p-*dioxin | 2 | -3471.819 | -1.038 | 0.069 | -25.520 |
| 1,2,4,6,9-pentabromo-7-chlorodibenzo*-p-*dioxin | 2 | -3472.003 | 0.020 | 0.001 | -25.764 |
| 1,2,4,6,9-pentabromo-8-chlorodibenzo*-p-*dioxin | 2 | -3472.002 | -0.728 | 0.031 | -25.098 |
| 1,2,4,7,8-pentabromo-3-chlorodibenzo*-p-*dioxin | 2 | -3471.899 | -0.060 | 0.005 | -25.733 |
| 1,2,4,7,8-pentabromo-6-chlorodibenzo*-p-*dioxin | 2 | -3472.002 | 0.612 | -0.036 | -25.947 |
| 1,2,4,7,8-pentabromo-9-chlorodibenzo*-p-*dioxin | 2 | -3472.002 | -0.607 | 0.007 | -24.709 |
| 1,2,4,7,9-pentabromo-3-chlorodibenzo*-p-*dioxin | 2 | -3471.889 | -0.680 | 0.042 | -25.497 |
| 1,2,4,7,9-pentabromo-6-chlorodibenzo*-p-*dioxin | 2 | -3472.000 | 0.021 | 0.002 | -25.792 |
| 1,2,4,7,9-pentabromo-8-chlorodibenzo*-p-*dioxin | 2 | -3471.907 | -0.538 | 0.007 | -24.860 |
| 1,2,4,8,9-pentabromo-3-chlorodibenzo*-p-*dioxin | 2 | -3471.829 | -1.715 | 0.062 | -24.028 |
| 1,2,4,8,9-pentabromo-6-chlorodibenzo*-p-*dioxin | 2 | -3472.085 | -0.663 | 0.028 | -25.130 |
| 1,2,4,8,9-pentabromo-7-chlorodibenzo*-p-*dioxin | 2 | -3472.002 | -0.475 | 0.003 | -24.860 |
| 1,2,3,4,6,7-hexabromodibenzo*-p-*dioxin | 2 | -3445.449 | 0.595 | 0.011 | -32.128 |
| 1,2,3,4,6,8-hexabromodibenzo*-p-*dioxin | 2 | -3445.509 | -0.270 | 0.027 | -30.861 |
| 1,2,3,4,6,9-hexabromodibenzo*-p-*dioxin | 2 | -3445.438 | -1.049 | 0.070 | -30.485 |
| 1,2,3,4,7,8-hexabromodibenzo*-p-*dioxin | 2 | -3445.518 | -0.072 | 0.007 | -30.722 |
| 1,2,3,6,7,8-hexabromodibenzo*-p-*dioxin | 2 | -3445.529 | 0.000 | 0.000 | -30.677 |
| 1,2,3,6,7,9-hexabromodibenzo*-p-*dioxin | 2 | -3445.526 | -0.572 | 0.036 | -30.508 |
| 1,2,3,6,8,9-hexabromodibenzo*-p-*dioxin | 2 | -3445.526 | -1.293 | 0.075 | -30.127 |
| 1,2,4,6,7,9-hexabromodibenzo*-p-*dioxin | 2 | -3445.524 | 0.000 | 0.001 | -30.704 |
| 1,2,4,6,8,9-hexabromodibenzo*-p-*dioxin | 2 | -3445.524 | -0.718 | 0.031 | -30.096 |
| 1,2,3,4,6,7,8-heptachlorodibenzo*-p-*dioxin | 1 | -3845.467 | 0.586 | -0.020 | -2.132 |
| 1-bromo-2,3,4,6,7,8-hexachlorodibenzo*-p-*dioxin | 1 | -3818.876 | 0.669 | -0.022 | -7.240 |
| 1-bromo-2,3,4,6,7,9-hexachlorodibenzo*-p-*dioxin | 1 | -3818.922 | 0.041 | 0.011 | -6.875 |
| 1-bromo-2,3,4,6,8,9-hexachlorodibenzo*-p-*dioxin | 1 | -3818.921 | -0.704 | 0.039 | -6.163 |
| 1-bromo-2,3,4,7,8,9-hexachlorodibenzo*-p-*dioxin | 1 | -3818.876 | -0.550 | 0.026 | -6.132 |
| 1-bromo-2,3,6,7,8,9-hexachlorodibenzo*-p-*dioxin | 1 | -3818.874 | -0.489 | 0.026 | -6.250 |
| 1-bromo-2,4,6,7,8,9-hexachlorodibenzo*-p-*dioxin | 1 | -3818.926 | 0.120 | -0.015 | -6.352 |
| 1-bromo-3,4,6,7,8,9-hexachlorodibenzo*-p-*dioxin | 1 | -3818.951 | 0.851 | -0.052 | -6.799 |
| 2-bromo-1,3,4,6,7,8-hexachlorodibenzo*-p-*dioxin | 1 | -3818.836 | 0.643 | -0.024 | -7.146 |
| 2-bromo-1,3,4,6,7,9-hexachlorodibenzo*-p-*dioxin | 1 | -3818.880 | 0.016 | 0.011 | -6.835 |
| 2-bromo-1,3,4,6,8,9-hexachlorodibenzo*-p-*dioxin | 1 | -3818.882 | -0.727 | 0.039 | -6.126 |
| 2-bromo-1,3,4,7,8,9-hexachlorodibenzo*-p-*dioxin | 1 | -3818.835 | -0.566 | 0.021 | -5.979 |
| 2-bromo-1,3,6,7,8,9-hexachlorodibenzo*-p-*dioxin | 1 | -3818.841 | -0.526 | 0.030 | -6.288 |
| 2-bromo-1,4,6,7,8,9-hexachlorodibenzo*-p-*dioxin | 1 | -3818.918 | 0.107 | -0.013 | -6.380 |
| 2-bromo-3,4,6,7,8,9-hexachlorodibenzo*-p-*dioxin | 1 | -3818.869 | 0.672 | -0.032 | -6.988 |
| 1,2-dibromo-3,4,6,7,8-pentachlorodibenzo*-p-*dioxin | 1 | -3792.361 | 0.675 | -0.022 | -12.238 |
| 1,2-dibromo-3,4,6,7,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.404 | 0.050 | 0.011 | -11.879 |
| 1,2-dibromo-3,4,6,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.405 | -0.692 | 0.036 | -11.095 |
| 1,2-dibromo-3,4,7,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.359 | -0.537 | 0.019 | -10.961 |
| 1,2-dibromo-3,6,7,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.362 | -0.482 | 0.024 | -11.197 |
| 1,2-dibromo-4,6,7,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.444 | 0.145 | -0.015 | -11.380 |
| 1,3-dibromo-2,4,6,7,8-pentachlorodibenzo*-p-*dioxin | 1 | -3792.234 | 0.655 | -0.023 | -12.197 |
| 1,3-dibromo-2,4,6,7,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.280 | 0.029 | 0.012 | -11.888 |
| 1,3-dibromo-2,4,6,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.278 | -0.712 | 0.041 | -11.210 |
| 1,3-dibromo-2,4,7,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.235 | -0.557 | 0.025 | -11.102 |
| 1,3-dibromo-2,6,7,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.266 | -0.504 | 0.026 | -11.224 |
| 1,3-dibromo-4,6,7,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.360 | 0.842 | -0.042 | -12.041 |
| 1,4-dibromo-2,3,6,7,8-pentachlorodibenzo*-p-*dioxin | 1 | -3792.280 | 0.585 | -0.017 | -12.209 |
| 1,4-dibromo-2,3,6,7,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.325 | -0.043 | 0.020 | -11.948 |
| 1,4-dibromo-2,6,7,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.361 | 0.031 | -0.016 | -11.149 |
| 1,6-dibromo-2,3,4,7,8-pentachlorodibenzo*-p-*dioxin | 1 | -3792.284 | 0.572 | -0.023 | -12.027 |
| 1,6-dibromo-2,3,4,7,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.337 | -0.034 | 0.014 | -11.807 |
| 1,6-dibromo-2,3,4,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.360 | -0.767 | 0.045 | -11.192 |
| 1,7-dibromo-2,3,4,6,8-pentachlorodibenzo*-p-*dioxin | 1 | -3792.250 | 0.611 | -0.021 | -12.161 |
| 1,7-dibromo-2,3,4,6,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.328 | -0.021 | 0.016 | -11.886 |
| 1,7-dibromo-2,3,4,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.277 | -0.593 | 0.023 | -10.972 |
| 1,7-dibromo-2,3,6,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.243 | -0.545 | 0.031 | -11.279 |
| 1,7-dibromo-2,4,6,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.294 | 0.061 | -0.014 | -11.272 |
| 1,7-dibromo-3,4,6,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.320 | 0.792 | -0.049 | -11.771 |
| 1,8-dibromo-2,3,4,6,7-pentachlorodibenzo*-p-*dioxin | 1 | -3792.278 | 0.688 | -0.025 | -12.201 |
| 1,8-dibromo-2,3,4,6,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.328 | -0.686 | 0.039 | -11.199 |
| 1,8-dibromo-2,3,4,7,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.251 | -0.526 | 0.024 | -11.133 |
| 1,8-dibromo-2,3,6,7,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.243 | -0.469 | 0.026 | -11.296 |
| 1,8-dibromo-2,4,6,7,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.296 | 0.138 | -0.013 | -11.446 |
| 1,8-dibromo-3,4,6,7,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.319 | 0.864 | -0.044 | -12.040 |
| 1,9-dibromo-2,3,4,6,7-pentachlorodibenzo*-p-*dioxin | 1 | -3792.361 | 0.115 | 0.005 | -11.857 |
| 1,9-dibromo-2,3,4,6,8-pentachlorodibenzo*-p-*dioxin | 1 | -3792.336 | -0.635 | 0.038 | -11.269 |
| 1,9-dibromo-2,3,4,7,8-pentachlorodibenzo*-p-*dioxin | 1 | -3792.285 | -0.461 | 0.021 | -11.174 |
| 2,3-dibromo-1,4,6,7,8-pentachlorodibenzo*-p-*dioxin | 1 | -3792.325 | 0.613 | -0.022 | -12.125 |
| 2,3-dibromo-1,4,6,7,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.370 | -0.013 | 0.011 | -11.764 |
| 2,3-dibromo-1,6,7,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.362 | -0.552 | 0.029 | -11.191 |
| 2,7-dibromo-1,3,4,6,8-pentachlorodibenzo*-p-*dioxin | 1 | -3792.211 | 0.585 | -0.021 | -12.118 |
| 2,7-dibromo-1,3,4,6,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.287 | -0.046 | 0.016 | -11.845 |
| 2,7-dibromo-1,3,4,8,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.237 | -0.610 | 0.024 | -10.973 |
| 2,8-dibromo-1,3,4,6,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.287 | -0.709 | 0.038 | -11.136 |
| 2,8-dibromo-1,3,4,7,9-pentachlorodibenzo*-p-*dioxin | 1 | -3792.208 | -0.544 | 0.020 | -11.002 |
| 1,2,3-tribromo-4,6,7,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.851 | 0.657 | -0.022 | -17.188 |
| 1,2,3-tribromo-4,6,7,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.897 | 0.033 | 0.010 | -16.805 |
| 1,2,3-tribromo-4,6,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.895 | -0.705 | 0.037 | -16.080 |
| 1,2,3-tribromo-4,7,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.851 | -0.549 | 0.020 | -15.948 |
| 1,2,3-tribromo-6,7,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.884 | -0.500 | 0.024 | -16.141 |
| 1,2,4-tribromo-3,6,7,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.755 | 0.589 | -0.014 | -17.282 |
| 1,2,4-tribromo-3,6,7,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.799 | -0.037 | 0.017 | -16.870 |
| 1,2,4-tribromo-3,6,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.800 | -0.784 | 0.039 | -15.997 |
| 1,2,4-tribromo-3,7,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.754 | -0.618 | 0.018 | -15.781 |
| 1,2,4-tribromo-6,7,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.882 | 0.055 | -0.015 | -16.201 |
| 1,2,6-tribromo-3,4,7,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.768 | 0.577 | -0.022 | -17.049 |
| 1,2,6-tribromo-3,4,7,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.819 | -0.028 | 0.015 | -16.831 |
| 1,2,6-tribromo-3,4,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.844 | -0.758 | 0.043 | -16.143 |
| 1,2,6-tribromo-3,7,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.771 | -0.567 | 0.033 | -16.266 |
| 1,2,6-tribromo-4,7,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.855 | 0.059 | -0.010 | -16.343 |
| 1,2,7-tribromo-3,4,6,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.735 | 0.618 | -0.021 | -17.160 |
| 1,2,7-tribromo-3,4,6,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.811 | -0.011 | 0.015 | -16.866 |
| 1,2,7-tribromo-3,4,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.761 | -0.579 | 0.022 | -15.959 |
| 1,2,7-tribromo-3,6,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.731 | -0.538 | 0.028 | -16.200 |
| 1,2,7-tribromo-4,6,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.813 | 0.087 | -0.016 | -16.250 |
| 1,2,8-tribromo-3,4,6,7-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.762 | 0.694 | -0.023 | -17.250 |
| 1,2,8-tribromo-3,4,6,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.811 | -0.674 | 0.037 | -16.156 |
| 1,2,8-tribromo-3,4,7,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.733 | -0.514 | 0.020 | -16.038 |
| 1,2,8-tribromo-3,6,7,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.730 | -0.463 | 0.025 | -16.267 |
| 1,2,8-tribromo-4,6,7,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.814 | 0.163 | -0.012 | -16.500 |
| 1,2,9-tribromo-3,4,6,7-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.844 | 0.126 | 0.003 | -16.812 |
| 1,2,9-tribromo-3,4,6,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.820 | -0.621 | 0.036 | -16.231 |
| 1,2,9-tribromo-3,4,7,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.768 | -0.445 | 0.019 | -16.139 |
| 1,2,9-tribromo-3,6,7,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.772 | -0.409 | 0.024 | -16.338 |
| 1,2,9-tribromo-4,6,7,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.855 | 0.219 | -0.017 | -16.471 |
| 1,3,6-tribromo-2,4,7,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.642 | 0.557 | -0.022 | -17.034 |
| 1,3,6-tribromo-2,4,7,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.696 | -0.047 | 0.022 | -16.999 |
| 1,3,6-tribromo-2,4,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.718 | -0.776 | 0.043 | -16.132 |
| 1,3,6-tribromo-2,7,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.677 | -0.588 | 0.034 | -16.269 |
| 1,3,6-tribromo-4,7,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.770 | 0.758 | -0.041 | -16.905 |
| 1,3,7-tribromo-2,4,6,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.607 | 0.597 | -0.022 | -17.118 |
| 1,3,7-tribromo-2,4,6,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.686 | -0.033 | 0.014 | -16.821 |
| 1,3,7-tribromo-2,4,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.636 | -0.600 | 0.023 | -15.968 |
| 1,3,7-tribromo-2,6,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.635 | -0.560 | 0.030 | -16.228 |
| 1,3,7-tribromo-4,6,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.729 | 0.783 | -0.048 | -16.779 |
| 1,3,8-tribromo-2,4,6,7-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.636 | 0.674 | -0.025 | -17.183 |
| 1,3,8-tribromo-2,4,6,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.686 | -0.694 | 0.041 | -16.245 |
| 1,3,8-tribromo-2,4,7,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.610 | -0.534 | 0.024 | -16.127 |
| 1,3,8-tribromo-2,6,7,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.636 | -0.485 | 0.026 | -16.268 |
| 1,3,8-tribromo-4,6,7,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.729 | 0.856 | -0.043 | -17.050 |
| 1,3,9-tribromo-2,4,6,7-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.720 | 0.102 | 0.004 | -16.815 |
| 1,3,9-tribromo-2,4,6,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.693 | -0.645 | 0.036 | -16.208 |
| 1,3,9-tribromo-2,4,7,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.643 | -0.470 | 0.021 | -16.166 |
| 1,3,9-tribromo-2,6,7,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.677 | -0.435 | 0.024 | -16.305 |
| 1,3,9-tribromo-4,6,7,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.770 | 0.917 | -0.046 | -17.082 |
| 1,4,6-tribromo-2,3,7,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.690 | 0.501 | -0.018 | -17.021 |
| 1,4,6-tribromo-2,3,7,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.742 | -0.106 | 0.021 | -16.851 |
| 1,4,6-tribromo-2,3,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.766 | -0.844 | 0.046 | -16.070 |
| 1,4,6-tribromo-2,7,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.772 | -0.042 | -0.010 | -16.164 |
| 1,4,6-tribromo-3,7,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.772 | 0.699 | -0.034 | -16.972 |
| 1,4,7-tribromo-2,3,6,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.655 | 0.525 | -0.015 | -17.152 |
| 1,4,7-tribromo-2,3,6,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.732 | -0.107 | 0.024 | -16.929 |
| 1,4,7-tribromo-2,3,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.682 | -0.673 | 0.024 | -15.845 |
| 1,4,7-tribromo-2,6,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.729 | -0.029 | -0.014 | -16.093 |
| 1,4,7-tribromo-3,6,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.730 | 0.709 | -0.045 | -16.714 |
| 1,7,8-tribromo-2,3,4,6-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.771 | 0.638 | -0.023 | -17.140 |
| 1,7,8-tribromo-2,3,4,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.771 | -0.569 | 0.025 | -16.055 |
| 1,7,8-tribromo-2,3,6,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.732 | -0.514 | 0.028 | -16.246 |
| 1,7,8-tribromo-2,4,6,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.784 | 0.090 | -0.014 | -16.313 |
| 1,7,8-tribromo-3,4,6,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.809 | 0.818 | -0.049 | -16.806 |
| 2,3,7-tribromo-1,4,6,8-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.699 | 0.553 | -0.020 | -17.068 |
| 2,3,7-tribromo-1,4,6,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.776 | -0.076 | 0.014 | -16.721 |
| 2,3,7-tribromo-1,4,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.726 | -0.634 | 0.026 | -15.963 |
| 2,3,7-tribromo-1,6,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.731 | -0.610 | 0.034 | -16.217 |
| 2,3,7-tribromo-4,6,8,9-tetrachlorodibenzo*-p-*dioxin | 1 | -3765.730 | 0.587 | -0.029 | -16.894 |
| 1,2,3,4-tetrabromo-6,7,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.373 | 0.572 | -0.013 | -22.236 |
| 1,2,3,4-tetrabromo-6,7,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.418 | -0.051 | 0.017 | -21.803 |
| 1,2,3,6-tetrabromo-4,7,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.260 | 0.558 | -0.020 | -22.049 |
| 1,2,3,6-tetrabromo-4,7,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.312 | -0.045 | 0.015 | -21.783 |
| 1,2,3,6-tetrabromo-4,8,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.335 | -0.771 | 0.042 | -21.077 |
| 1,2,3,6-tetrabromo-7,8,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.295 | -0.585 | 0.031 | -21.158 |
| 1,2,3,7-tetrabromo-4,6,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.225 | 0.599 | -0.021 | -22.109 |
| 1,2,3,7-tetrabromo-4,6,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.302 | -0.028 | 0.014 | -21.791 |
| 1,2,3,7-tetrabromo-4,8,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.252 | -0.591 | 0.021 | -20.895 |
| 1,2,3,7-tetrabromo-6,8,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.253 | -0.556 | 0.030 | -21.196 |
| 1,2,3,8-tetrabromo-4,6,7-trichlorodibenzo*-p-*dioxin | 1 | -3739.253 | 0.676 | -0.024 | -22.174 |
| 1,2,3,8-tetrabromo-4,6,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.302 | -0.687 | 0.038 | -21.141 |
| 1,2,3,8-tetrabromo-4,7,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.226 | -0.525 | 0.020 | -21.001 |
| 1,2,3,8-tetrabromo-6,7,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.253 | -0.480 | 0.024 | -21.187 |
| 1,2,3,9-tetrabromo-4,6,7-trichlorodibenzo*-p-*dioxin | 1 | -3739.336 | 0.108 | 0.006 | -21.840 |
| 1,2,3,9-tetrabromo-4,6,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.311 | -0.636 | 0.035 | -21.160 |
| 1,2,3,9-tetrabromo-4,7,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.259 | -0.459 | 0.019 | -21.097 |
| 1,2,3,9-tetrabromo-6,7,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.295 | -0.428 | 0.024 | -21.280 |
| 1,2,4,6-tetrabromo-3,7,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.164 | 0.503 | -0.016 | -22.064 |
| 1,2,4,6-tetrabromo-3,7,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.215 | -0.102 | 0.021 | -21.847 |
| 1,2,4,6-tetrabromo-3,8,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.240 | -0.837 | 0.042 | -20.967 |
| 1,2,4,6-tetrabromo-7,8,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.293 | -0.020 | -0.010 | -21.185 |
| 1,2,4,7-tetrabromo-3,6,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.130 | 0.530 | -0.013 | -22.201 |
| 1,2,4,7-tetrabromo-3,6,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.206 | -0.100 | 0.023 | -21.904 |
| 1,2,4,7-tetrabromo-3,8,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.156 | -0.662 | 0.022 | -20.802 |
| 1,2,4,7-tetrabromo-6,8,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.251 | -0.005 | -0.012 | -21.170 |
| 1,2,4,8-tetrabromo-3,6,7-trichlorodibenzo*-p-*dioxin | 1 | -3739.156 | 0.609 | -0.016 | -22.271 |
| 1,2,4,8-tetrabromo-3,6,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.206 | -0.765 | 0.041 | -21.087 |
| 1,2,4,8-tetrabromo-3,7,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.127 | -0.593 | 0.018 | -20.837 |
| 1,2,4,8-tetrabromo-6,7,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.251 | 0.073 | -0.016 | -21.217 |
| 1,2,4,9-tetrabromo-3,6,7-trichlorodibenzo*-p-*dioxin | 1 | -3739.239 | 0.039 | 0.011 | -21.855 |
| 1,2,4,9-tetrabromo-3,6,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.217 | -0.713 | 0.037 | -21.081 |
| 1,2,4,9-tetrabromo-3,7,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.164 | -0.527 | 0.020 | -21.009 |
| 1,2,4,9-tetrabromo-6,7,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.293 | 0.128 | -0.016 | -21.316 |
| 1,2,6,7-tetrabromo-3,4,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.256 | 0.573 | -0.021 | -22.053 |
| 1,2,6,7-tetrabromo-3,4,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.338 | -0.051 | 0.017 | -21.818 |
| 1,2,6,8-tetrabromo-3,4,7-trichlorodibenzo*-p-*dioxin | 1 | -3739.160 | 0.593 | -0.021 | -22.109 |
| 1,2,6,8-tetrabromo-3,4,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.253 | -0.747 | 0.043 | -21.164 |
| 1,2,6,8-tetrabromo-3,7,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.129 | -0.552 | 0.032 | -21.279 |
| 1,2,6,8-tetrabromo-4,7,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.214 | 0.072 | -0.011 | -21.352 |
| 1,2,6,9-tetrabromo-3,4,7-trichlorodibenzo*-p-*dioxin | 1 | -3739.255 | 0.050 | 0.007 | -21.769 |
| 1,2,6,9-tetrabromo-3,4,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.255 | -0.686 | 0.039 | -21.178 |
| 1,2,6,9-tetrabromo-3,7,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.177 | -0.494 | 0.029 | -21.304 |
| 1,2,6,9-tetrabromo-4,7,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.260 | 0.133 | -0.011 | -21.461 |
| 1,2,7,8-tetrabromo-3,4,6-trichlorodibenzo*-p-*dioxin | 1 | -3739.255 | 0.645 | -0.021 | -22.192 |
| 1,2,7,8-tetrabromo-3,4,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.254 | -0.556 | 0.023 | -21.014 |
| 1,2,7,8-tetrabromo-3,6,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.219 | -0.507 | 0.027 | -21.219 |
| 1,2,7,8-tetrabromo-4,6,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.302 | 0.116 | -0.014 | -21.343 |
| 1,2,7,9-tetrabromo-3,4,6-trichlorodibenzo*-p-*dioxin | 1 | -3739.254 | 0.064 | 0.007 | -21.797 |
| 1,2,7,9-tetrabromo-3,4,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.160 | -0.485 | 0.022 | -21.143 |
| 1,2,7,9-tetrabromo-3,6,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.131 | -0.466 | 0.026 | -21.289 |
| 1,2,7,9-tetrabromo-4,6,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.212 | 0.160 | -0.014 | -21.445 |
| 1,2,8,9-tetrabromo-3,4,6-trichlorodibenzo*-p-*dioxin | 1 | -3739.338 | -0.609 | 0.033 | -21.156 |
| 1,2,8,9-tetrabromo-3,4,7-trichlorodibenzo*-p-*dioxin | 1 | -3739.255 | -0.425 | 0.018 | -21.137 |
| 1,3,6,8-tetrabromo-2,4,7-trichlorodibenzo*-p-*dioxin | 1 | -3739.036 | 0.574 | -0.024 | -22.018 |
| 1,3,6,8-tetrabromo-2,4,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.129 | -0.767 | 0.045 | -21.201 |
| 1,3,6,9-tetrabromo-2,4,7-trichlorodibenzo*-p-*dioxin | 1 | -3739.132 | 0.028 | 0.007 | -21.750 |
| 1,3,6,9-tetrabromo-2,4,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.130 | -0.709 | 0.041 | -21.209 |
| 1,3,6,9-tetrabromo-2,7,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.082 | -0.519 | 0.031 | -21.326 |
| 1,3,6,9-tetrabromo-4,7,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.175 | 0.833 | -0.045 | -21.947 |
| 1,3,7,8-tetrabromo-2,4,6-trichlorodibenzo*-p-*dioxin | 1 | -3739.129 | 0.624 | -0.023 | -22.123 |
| 1,3,7,8-tetrabromo-2,4,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.130 | -0.576 | 0.025 | -21.051 |
| 1,3,7,8-tetrabromo-2,6,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.124 | -0.530 | 0.029 | -21.244 |
| 1,3,7,8-tetrabromo-4,6,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.218 | 0.808 | -0.050 | -21.761 |
| 1,3,7,9-tetrabromo-2,4,6-trichlorodibenzo*-p-*dioxin | 1 | -3739.128 | 0.039 | 0.009 | -21.824 |
| 1,3,7,9-tetrabromo-2,4,8-trichlorodibenzo*-p-*dioxin | 1 | -3739.035 | -0.510 | 0.022 | -21.118 |
| 1,4,6,9-tetrabromo-2,3,7-trichlorodibenzo*-p-*dioxin | 1 | -3739.178 | -0.029 | 0.018 | -21.917 |
| 1,4,7,8-tetrabromo-2,3,6-trichlorodibenzo*-p-*dioxin | 1 | -3739.176 | 0.554 | -0.017 | -22.135 |
| 1,4,7,8-tetrabromo-2,6,9-trichlorodibenzo*-p-*dioxin | 1 | -3739.219 | 0.002 | -0.013 | -21.164 |
| 2,3,7,8-tetrabromo-1,4,6-trichlorodibenzo*-p-*dioxin | 1 | -3739.219 | 0.580 | -0.022 | -22.047 |
| 1,2,3,4,6-pentabromo-7,8-dichlorodibenzo*-p-*dioxin | 1 | -3712.783 | 0.485 | -0.015 | -27.016 |
| 1,2,3,4,6-pentabromo-7,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.834 | -0.117 | 0.022 | -26.804 |
| 1,2,3,4,6-pentabromo-8,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.858 | -0.846 | 0.044 | -25.962 |
| 1,2,3,4,7-pentabromo-6,8-dichlorodibenzo*-p-*dioxin | 1 | -3712.748 | 0.513 | -0.013 | -27.129 |
| 1,2,3,4,7-pentabromo-6,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.824 | -0.113 | 0.023 | -26.840 |
| 1,2,3,4,7-pentabromo-8,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.775 | -0.672 | 0.022 | -25.743 |
| 1,2,3,6,7-pentabromo-4,8-dichlorodibenzo*-p-*dioxin | 1 | -3712.747 | 0.553 | -0.022 | -26.973 |
| 1,2,3,6,7-pentabromo-4,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.830 | -0.068 | 0.017 | -26.770 |
| 1,2,3,6,7-pentabromo-8,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.778 | -0.589 | 0.033 | -26.188 |
| 1,2,3,6,8-pentabromo-4,7-dichlorodibenzo*-p-*dioxin | 1 | -3712.652 | 0.575 | -0.021 | -27.059 |
| 1,2,3,6,8-pentabromo-4,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.745 | -0.761 | 0.045 | -26.174 |
| 1,2,3,6,8-pentabromo-7,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.653 | -0.570 | 0.032 | -26.223 |
| 1,2,3,6,9-pentabromo-4,7-dichlorodibenzo*-p-*dioxin | 1 | -3712.747 | 0.033 | 0.008 | -26.747 |
| 1,2,3,6,9-pentabromo-4,8-dichlorodibenzo*-p-*dioxin | 1 | -3712.746 | -0.702 | 0.040 | -26.158 |
| 1,2,3,6,9-pentabromo-7,8-dichlorodibenzo*-p-*dioxin | 1 | -3712.700 | -0.513 | 0.030 | -26.272 |
| 1,2,3,7,8-pentabromo-4,6-dichlorodibenzo*-p-*dioxin | 1 | -3712.746 | 0.626 | -0.022 | -27.114 |
| 1,2,3,7,8-pentabromo-4,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.746 | -0.568 | 0.024 | -26.001 |
| 1,2,3,7,8-pentabromo-6,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.742 | -0.525 | 0.027 | -26.163 |
| 1,2,3,7,9-pentabromo-4,6-dichlorodibenzo*-p-*dioxin | 1 | -3712.745 | 0.046 | 0.009 | -26.798 |
| 1,2,3,7,9-pentabromo-4,8-dichlorodibenzo*-p-*dioxin | 1 | -3712.651 | -0.499 | 0.022 | -26.101 |
| 1,2,3,7,9-pentabromo-6,8-dichlorodibenzo*-p-*dioxin | 1 | -3712.653 | -0.485 | 0.028 | -26.283 |
| 1,2,3,8,9-pentabromo-4,6-dichlorodibenzo*-p-*dioxin | 1 | -3712.829 | -0.623 | 0.035 | -26.165 |
| 1,2,3,8,9-pentabromo-4,7-dichlorodibenzo*-p-*dioxin | 1 | -3712.747 | -0.438 | 0.017 | -26.071 |
| 1,2,3,8,9-pentabromo-6,7-dichlorodibenzo*-p-*dioxin | 1 | -3712.778 | -0.411 | 0.022 | -26.247 |
| 1,2,4,6,7-pentabromo-3,8-dichlorodibenzo*-p-*dioxin | 1 | -3712.652 | 0.497 | -0.015 | -27.064 |
| 1,2,4,6,7-pentabromo-3,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.733 | -0.127 | 0.020 | -26.752 |
| 1,2,4,6,7-pentabromo-8,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.776 | -0.029 | -0.011 | -26.128 |
| 1,2,4,6,8-pentabromo-3,7-dichlorodibenzo*-p-*dioxin | 1 | -3712.556 | 0.521 | -0.016 | -27.102 |
| 1,2,4,6,8-pentabromo-3,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.649 | -0.825 | 0.045 | -26.068 |
| 1,2,4,6,8-pentabromo-7,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.652 | -0.006 | -0.010 | -26.222 |
| 1,2,4,6,9-pentabromo-3,7-dichlorodibenzo*-p-*dioxin | 1 | -3712.652 | -0.023 | 0.012 | -26.760 |
| 1,2,4,6,9-pentabromo-3,8-dichlorodibenzo*-p-*dioxin | 1 | -3712.653 | -0.766 | 0.043 | -26.130 |
| 1,2,4,6,9-pentabromo-7,8-dichlorodibenzo*-p-*dioxin | 1 | -3712.699 | 0.054 | -0.007 | -26.407 |
| 1,2,4,7,8-pentabromo-3,6-dichlorodibenzo*-p-*dioxin | 1 | -3712.651 | 0.558 | -0.015 | -27.182 |
| 1,2,4,7,8-pentabromo-3,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.649 | -0.637 | 0.021 | -25.808 |
| 1,2,4,7,8-pentabromo-6,9-dichlorodibenzo*-p-*dioxin | 1 | -3712.740 | 0.025 | -0.013 | -26.187 |
| 1,2,4,7,9-pentabromo-3,6-dichlorodibenzo*-p-*dioxin | 1 | -3712.650 | -0.024 | 0.015 | -26.837 |
| 1,2,4,7,9-pentabromo-3,8-dichlorodibenzo*-p-*dioxin | 1 | -3712.556 | -0.568 | 0.023 | -26.011 |
| 1,2,4,7,9-pentabromo-6,8-dichlorodibenzo*-p-*dioxin | 1 | -3712.651 | 0.068 | -0.014 | -26.261 |
| 1,2,4,8,9-pentabromo-3,6-dichlorodibenzo*-p-*dioxin | 1 | -3712.734 | -0.699 | 0.036 | -26.062 |
| 1,2,4,8,9-pentabromo-3,7-dichlorodibenzo*-p-*dioxin | 1 | -3712.650 | -0.504 | 0.019 | -26.013 |
| 1,2,4,8,9-pentabromo-6,7-dichlorodibenzo*-p-*dioxin | 1 | -3712.776 | 0.144 | -0.015 | -26.359 |
| 1,2,3,4,6,7-hexabromo-8-chlorodibenzo*-p-*dioxin | 1 | -3686.270 | 0.479 | -0.015 | -31.990 |
| 1,2,3,4,6,7-hexabromo-9-chlorodibenzo*-p-*dioxin | 1 | -3686.352 | -0.142 | 0.024 | -31.787 |
| 1,2,3,4,6,8-hexabromo-7-chlorodibenzo*-p-*dioxin | 1 | -3686.175 | 0.503 | -0.016 | -32.028 |
| 1,2,3,4,6,8-hexabromo-9-chlorodibenzo*-p-*dioxin | 1 | -3686.268 | -0.835 | 0.046 | -31.036 |
| 1,2,3,4,7,8-hexabromo-6-chlorodibenzo*-p-*dioxin | 1 | -3686.268 | 0.541 | -0.015 | -32.110 |
| 1,2,3,6,7,8-hexabromo-4-chlorodibenzo*-p-*dioxin | 1 | -3686.270 | 0.571 | -0.023 | -31.960 |
| 1,2,3,6,7,9-hexabromo-4-chlorodibenzo*-p-*dioxin | 1 | -3686.268 | 0.011 | 0.011 | -31.761 |
| 1,2,3,6,7,9-hexabromo-8-chlorodibenzo*-p-*dioxin | 1 | -3686.174 | -0.515 | 0.030 | -31.256 |
| 1,2,3,6,8,9-hexabromo-4-chlorodibenzo*-p-*dioxin | 1 | -3686.268 | -0.693 | 0.041 | -31.180 |
| 1,2,3,6,8,9-hexabromo-7-chlorodibenzo*-p-*dioxin | 1 | -3686.174 | -0.498 | 0.029 | -31.263 |
| 1,2,3,7,8,9-hexabromo-4-chlorodibenzo*-p-*dioxin | 1 | -3686.269 | -0.481 | 0.021 | -31.070 |
| 1,2,4,6,7,9-hexabromo-3-chlorodibenzo*-p-*dioxin | 1 | -3686.173 | -0.047 | 0.016 | -31.797 |
| 1,2,4,6,8,9-hexabromo-3-chlorodibenzo*-p-*dioxin | 1 | -3686.173 | -0.756 | 0.042 | -31.102 |
| 1,2,3,4,6,7,9-heptabromodibenzo*-p-*dioxin | 1 | -3659.791 | -0.063 | 0.017 | -36.753 |
| 1,2,3,4,6,7,8,9-octochlorodibenzo*-p-*dioxin | 0 | -4086.242 | 0.000 | 0.001 | -2.315 |
| 1-bromo-2,3,4,6,7,8,9-heptachlorodibenzo*-p-*dioxin | 0 | -4059.651 | 0.086 | -0.004 | -7.352 |
| 2-bromo-1,3,4,6,7,8,9-heptachlorodibenzo*-p-*dioxin | 0 | -4059.610 | 0.061 | -0.004 | -7.311 |
| 1,2-dibromo-3,4,6,7,8,9-hexachlorodibenzo*-p-*dioxin | 0 | -4033.134 | 0.098 | -0.004 | -12.361 |
| 1,3-dibromo-2,4,6,7,8,9-hexachlorodibenzo*-p-*dioxin | 0 | -4033.009 | 0.076 | -0.002 | -12.394 |
| 1,4-dibromo-2,3,6,7,8,9-hexachlorodibenzo*-p-*dioxin | 0 | -4033.055 | 0.002 | 0.000 | -12.294 |
| 1,6-dibromo-2,3,4,7,8,9-hexachlorodibenzo*-p-*dioxin | 0 | -4033.062 | 0.000 | 0.002 | -12.341 |
| 1,8-dibromo-2,3,4,6,7,9-hexachlorodibenzo*-p-*dioxin | 0 | -4033.020 | 0.103 | -0.001 | -12.470 |
| 1,9-dibromo-2,3,4,6,7,8-hexachlorodibenzo*-p-*dioxin | 0 | -4033.062 | 0.158 | -0.005 | -12.465 |
| 2,3-dibromo-1,4,6,7,8,9-hexachlorodibenzo*-p-*dioxin | 0 | -4033.099 | 0.033 | -0.001 | -12.320 |
| 2,7-dibromo-1,3,4,6,8,9-hexachlorodibenzo*-p-*dioxin | 0 | -4032.980 | 0.000 | 0.000 | -12.305 |
| 2,8-dibromo-1,3,4,6,7,9-hexachlorodibenzo*-p-*dioxin | 0 | -4032.978 | 0.077 | -0.002 | -12.402 |
| 1,2,3-tribromo-4,6,7,8,9-pentachlorodibenzo*-p-*dioxin | 0 | -4006.625 | 0.082 | -0.004 | -17.315 |
| 1,2,4-tribromo-3,6,7,8,9-pentachlorodibenzo*-p-*dioxin | 0 | -4006.529 | 0.011 | 0.001 | -17.326 |
| 1,2,6-tribromo-3,4,7,8,9-pentachlorodibenzo*-p-*dioxin | 0 | -4006.544 | 0.009 | 0.000 | -17.293 |
| 1,2,7-tribromo-3,4,6,8,9-pentachlorodibenzo*-p-*dioxin | 0 | -4006.503 | 0.039 | -0.001 | -17.333 |
| 1,2,8-tribromo-3,4,6,7,9-pentachlorodibenzo*-p-*dioxin | 0 | -4006.503 | 0.114 | -0.003 | -17.426 |
| 1,2,9-tribromo-3,4,6,7,8-pentachlorodibenzo*-p-*dioxin | 0 | -4006.545 | 0.172 | -0.007 | -17.426 |
| 1,3,6-tribromo-2,4,7,8,9-pentachlorodibenzo*-p-*dioxin | 0 | -4006.420 | -0.012 | 0.002 | -17.327 |
| 1,3,7-tribromo-2,4,6,8,9-pentachlorodibenzo*-p-*dioxin | 0 | -4006.377 | 0.016 | -0.002 | -17.286 |
| 1,3,8-tribromo-2,4,6,7,9-pentachlorodibenzo*-p-*dioxin | 0 | -4006.379 | 0.093 | -0.001 | -17.460 |
| 1,3,9-tribromo-2,4,6,7,8-pentachlorodibenzo*-p-*dioxin | 0 | -4006.420 | 0.145 | -0.007 | -17.397 |
| 1,4,6-tribromo-2,3,7,8,9-pentachlorodibenzo*-p-*dioxin | 0 | -4006.467 | -0.071 | 0.004 | -17.257 |
| 1,4,7-tribromo-2,3,6,8,9-pentachlorodibenzo*-p-*dioxin | 0 | -4006.424 | -0.060 | 0.005 | -17.312 |
| 1,7,8-tribromo-2,3,4,6,9-pentachlorodibenzo*-p-*dioxin | 0 | -4006.509 | 0.055 | -0.001 | -17.362 |
| 2,3,7-tribromo-1,4,6,8,9-pentachlorodibenzo*-p-*dioxin | 0 | -4006.467 | -0.028 | 0.002 | -17.288 |
| 1,2,3,4-tetrabromo-6,7,8,9-tetrachlorodibenzo*-p-*dioxin | 0 | -3980.147 | -0.002 | 0.000 | -22.235 |
| 1,2,3,7-tetrabromo-4,6,8,9-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.994 | 0.022 | -0.001 | -22.285 |
| 1,2,3,8-tetrabromo-4,6,7,9-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.995 | 0.098 | -0.002 | -22.405 |
| 1,2,3,9-tetrabromo-4,6,7,8-tetrachlorodibenzo*-p-*dioxin | 0 | -3980.036 | 0.154 | -0.007 | -22.376 |
| 1,2,4,6-tetrabromo-3,7,8,9-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.941 | -0.064 | 0.003 | -22.232 |
| 1,2,4,7-tetrabromo-3,6,8,9-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.898 | -0.050 | 0.003 | -22.267 |
| 1,2,4,8-tetrabromo-3,6,7,9-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.897 | 0.029 | 0.001 | -22.368 |
| 1,2,4,9-tetrabromo-3,6,7,8-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.941 | 0.085 | -0.001 | -22.416 |
| 1,2,6,7-tetrabromo-3,4,8,9-tetrachlorodibenzo*-p-*dioxin | 0 | -3980.027 | 0.000 | 0.003 | -22.340 |
| 1,2,6,8-tetrabromo-3,4,7,9-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.902 | 0.021 | 0.002 | -22.378 |
| 1,2,6,9-tetrabromo-3,4,7,8-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.950 | 0.083 | -0.002 | -22.385 |
| 1,2,7,8-tetrabromo-3,4,6,9-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.992 | 0.067 | -0.002 | -22.346 |
| 1,2,7,9-tetrabromo-3,4,6,8-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.903 | 0.112 | -0.003 | -22.423 |
| 1,2,8,9-tetrabromo-3,4,6,7-tetrachlorodibenzo*-p-*dioxin | 0 | -3980.028 | 0.185 | -0.005 | -22.489 |
| 1,3,6,8-tetrabromo-2,4,7,9-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.780 | 0.000 | 0.003 | -22.386 |
| 1,3,6,9-tetrabromo-2,4,7,8-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.826 | 0.057 | -0.001 | -22.384 |
| 1,3,7,8-tetrabromo-2,4,6,9-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.867 | 0.044 | -0.002 | -22.325 |
| 1,3,7,9-tetrabromo-2,4,6,8-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.777 | 0.085 | -0.003 | -22.395 |
| 1,4,6,9-tetrabromo-2,3,7,8-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.874 | 0.000 | 0.002 | -22.342 |
| 1,4,7,8-tetrabromo-2,3,6,9-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.913 | -0.029 | 0.002 | -22.279 |
| 2,3,7,8-tetrabromo-1,4,6,9-tetrachlorodibenzo*-p-*dioxin | 0 | -3979.956 | 0.000 | 0.002 | -22.327 |
| 1,2,3,4,6-pentabromo-7,8,9-trichlorodibenzo*-p-*dioxin | 0 | -3953.559 | -0.079 | 0.005 | -27.216 |
| 1,2,3,4,7-pentabromo-6,8,9-trichlorodibenzo*-p-*dioxin | 0 | -3953.516 | -0.064 | 0.003 | -27.201 |
| 1,2,3,6,7-pentabromo-4,8,9-trichlorodibenzo*-p-*dioxin | 0 | -3953.519 | -0.017 | 0.001 | -27.239 |
| 1,2,3,6,8-pentabromo-4,7,9-trichlorodibenzo*-p-*dioxin | 0 | -3953.395 | 0.005 | 0.001 | -27.305 |
| 1,2,3,6,9-pentabromo-4,7,8-trichlorodibenzo*-p-*dioxin | 0 | -3953.442 | 0.065 | -0.003 | -27.308 |
| 1,2,3,7,8-pentabromo-4,6,9-trichlorodibenzo*-p-*dioxin | 0 | -3953.483 | 0.051 | -0.001 | -27.326 |
| 1,2,3,7,9-pentabromo-4,6,8-trichlorodibenzo*-p-*dioxin | 0 | -3953.394 | 0.094 | -0.003 | -27.373 |
| 1,2,3,8,9-pentabromo-4,6,7-trichlorodibenzo*-p-*dioxin | 0 | -3953.519 | 0.168 | -0.005 | -27.441 |
| 1,2,4,6,7-pentabromo-3,8,9-trichlorodibenzo*-p-*dioxin | 0 | -3953.424 | -0.077 | 0.003 | -27.193 |
| 1,2,4,6,8-pentabromo-3,7,9-trichlorodibenzo*-p-*dioxin | 0 | -3953.298 | -0.050 | 0.004 | -27.295 |
| 1,2,4,6,9-pentabromo-3,7,8-trichlorodibenzo*-p-*dioxin | 0 | -3953.348 | 0.010 | 0.003 | -27.376 |
| 1,2,4,7,8-pentabromo-3,6,9-trichlorodibenzo*-p-*dioxin | 0 | -3953.387 | -0.019 | 0.004 | -27.338 |
| 1,2,4,7,9-pentabromo-3,6,8-trichlorodibenzo*-p-*dioxin | 0 | -3953.300 | 0.023 | -0.001 | -27.306 |
| 1,2,4,8,9-pentabromo-3,6,7-trichlorodibenzo*-p-*dioxin | 0 | -3953.423 | 0.100 | -0.001 | -27.431 |
| 1,2,3,4,6,7-hexabromo-8,9-dichlorodibenzo*-p-*dioxin | 0 | -3927.041 | -0.090 | 0.004 | -32.155 |
| 1,2,3,4,6,9-hexabromo-7,8-dichlorodibenzo*-p-*dioxin | 0 | -3926.966 | -0.007 | 0.002 | -32.278 |
| 1,2,3,4,7,8-hexabromo-6,9-dichlorodibenzo*-p-*dioxin | 0 | -3927.005 | -0.033 | 0.002 | -32.220 |
| 1,2,3,6,7,8-hexabromo-4,9-dichlorodibenzo*-p-*dioxin | 0 | -3927.010 | 0.000 | 0.001 | -32.257 |
| 1,2,3,6,7,9-hexabromo-4,8-dichlorodibenzo*-p-*dioxin | 0 | -3926.915 | 0.058 | -0.002 | -32.309 |
| 1,2,3,6,8,9-hexabromo-4,7-dichlorodibenzo*-p-*dioxin | 0 | -3926.915 | 0.076 | -0.003 | -32.318 |
| 1,2,3,7,8,9-hexabromo-4,6-dichlorodibenzo*-p-*dioxin | 0 | -3927.010 | 0.117 | -0.005 | -32.327 |
| 1,2,4,6,7,9-hexabromo-3,8-dichlorodibenzo*-p-*dioxin | 0 | -3926.821 | 0.000 | 0.001 | -32.292 |
| 1,2,4,6,8,9-hexabromo-3,7-dichlorodibenzo*-p-*dioxin | 0 | -3926.820 | 0.023 | 0.000 | -32.311 |
| 1,2,3,4,6,7,8-heptabromo-9-chlorodibenzo*-p-*dioxin | 0 | -3900.533 | -0.072 | 0.006 | -37.226 |
| 1,2,3,4,6,7,9-heptabromo-8-chlorodibenzo*-p-*dioxin | 0 | -3900.439 | -0.016 | 0.001 | -37.222 |

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