NAME

       MMFF94AtomTypes

SYNOPSIS

       use AtomTypes::MMFF94AtomTypes;

       use AtomTypes::MMFF94AtomTypes qw(:all);

DESCRIPTION

       MMFF94AtomTypes class provides the following methods:

       new, AssignAtomTypes, GetAllPossibleMMFF94AtomTypes, GetAllPossibleMMFF94NonHydrogenAtomTypes, GetMMFF94AtomTypesData, StringifyMMFF94AtomTypes

       The following functions are available:

       GetAllPossibleMMFF94AtomTypes, GetAllPossibleMMFF94NonHydrogenAtomTypes, GetMMFF94AtomTypesData

       MMFF94AtomTypes is derived from AtomTypes class which in turn is derived from ObjectProperty base class that provides methods not explicitly defined in MMFF94AtomTypes, AtomTypes or ObjectProperty classes using Perl's AUTOLOAD functionality. These methods are generated on-the-fly for a specified object property:

```
Set<PropertyName>(<PropertyValue>);
$PropertyValue = Get<PropertyName>();
Delete<PropertyName>();
```

       The data file MMFF94AtomTypes.csv distributed with MayaChemTools release contains all possible MMFF94 [Ref 83-87] atom types.

       Examples of MMFF94 atom types:

```
CR, C=C, C=N, C=S, NR, N=C, OR, OC=O and so on
```

METHODS

       new

```
$NewMMFF94AtomTypes = new AtomTypes::MMFF94AtomTypes(%NamesAndValues);
```

       Using specified *MMFF94AtomTypes* property names and values hash, new method creates a new object and returns a reference to newly created MMFF94AtomTypes object. By default, the following properties are initialized:

```
Molecule = ''
Type = 'MMFF94'
IgnoreHydrogens = 0
```

       Examples:

```
$MMFF94AtomTypes = new AtomTypes::MMFF94AtomTypes(
                            'Molecule' => $Molecule,
                            'IgnoreHydrogens' => 0);
```

       AssignAtomTypes

```
$MMFF94AtomTypes->AssignAtomTypes();
```

       Assigns MMFF94 atom types to all the atoms in a molecule and returns *MMFF94AtomTypes*.

       GetAllPossibleMMFF94AtomTypes

```
$AllAtomTypesDataRef = $MMFF94AtomTypes->
                    GetAllPossibleMMFF94AtomTypes();
$AllAtomTypesDataRef = AtomTypes::MMFF94AtomTypes::
                    GetAllPossibleMMFF94AtomTypes();
```

       Returns all possible MMFF94 atom types corresponding to hydrogen and non-hydrogen atoms as an array reference.

       GetAllPossibleMMFF94NonHydrogenAtomTypes

```
$AtomTypesDataRef = $MMFF94AtomTypes->
                       GetAllPossibleMMFF94NonHydrogenAtomTypes();
$AtomTypesDataRef = AtomTypes::MMFF94AtomTypes::
                       GetAllPossibleMMFF94NonHydrogenAtomTypes();
```

Returns all possible MMFF94 atom types corresponding to non-hydrogen atoms as an array reference.

GetMMFF94AtomTypesData

```
$AtomTypesDataMapRef = $MMFF94AtomTypes->GetMMFF94AtomTypesData();
$AtomTypesDataMapRef = AtomTypes::MMFF94AtomTypes::
                         GetMMFF94AtomTypesData();
```

Returns MMFF94 atom types and associated data loaded from MMFF94 data file as a reference to hash with the following hash data format:

```
@{$MMFF94AtomTypesDataMap{AtomTypes}} - Array of all possible atom
                           types for all atoms
@{$MMFF94AtomTypesDataMap{NonHydrogenAtomTypes}} - Array of all
                           possible atom types for non-hydrogen atoms
@{$MMFF94AtomTypesDataMap->{ColLabels}} - Array of column labels
%{$MMFF94AtomTypesDataMap->{DataCol<Num>}} - Hash keys pair:
                                    DataCol<Num>, AtomType
```

StringifyMMFF94AtomTypes

```
$String = $MMFF94AtomTypes->StringifyMMFF94AtomTypes();
```

Returns a string containing information about *MMFF94AtomTypes* object.

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SEE ALSO

AtomTypes.pm, AtomicInvariantsAtomTypes.pm, DREIDINGAtomTypes.pm, EStateAtomTypes.pm, FunctionalClassAtomTypes.pm, SLogPAtomTypes.pm, SYBYLAtomTypes.pm, TPSAAtomTypes.pm, UFFAtomTypes.pm

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