NAME

TPSAAtomTypes

SYNOPSIS

use AtomTypes::TPSAAtomTypes;

use AtomTypes::TPSAAtomTypes qw(:all);

DESCRIPTION

TPSAAtomTypes class provides the following methods:

new, AssignAtomTypes, GetAllPossibleTPSAAtomTypes, GetTPSAAtomTypesData, StringifyTPSAAtomTypes

The following functions are available:

GetAllPossibleTPSAAtomTypes, GetTPSAAtomTypesData

TPSAAtomTypes is derived from AtomTypes class which in turn is derived from ObjectProperty base class that provides methods not explicitly defined in TPSAAtomTypes, 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 TPSAAomTypes.csv distributed with MayaChemTools release contains all possible topological surface area (TPSA) [Ref 90-91] atom types.

The atom type symbols assigned by MayaChemTools are not used in the original publication and the numbers in atom symbols for element types simply correspond to their order of appearance in Table 1 [Ref 90].

Examples of TPSA atom types:

```
N1, N2, N3, O1, O2, O3, S1, S2, P1, P2 and so on
```

METHODS

new

```
$NewTPSAAtomTypes = new AtomTypes::TPSAAtomTypes(%NamesAndValues);
```

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

```
Molecule = ''
Type = 'TPSA'
IgnorePhosphorus = 0
IgnoreSulfur = 0
```

Examples:

```
$TPSAAtomTypes = new AtomTypes::TPSAAtomTypes(
                          'Molecule' => $Molecule,
                          'IgnorePhosphorus' => 0,
                          'IgnoreSulfur' => 0);
```

AssignAtomTypes

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

Assigns TPSA atom types to all the atoms in a molecule and returns *TPSAAtomTypes*.

GetAllPossibleTPSAAtomTypes

```
$AllAtomTypesDataRef = $TPSAAtomTypes->
                       GetAllPossibleTPSAAtomTypes();
```

```
$AllAtomTypesDataRef = AtomTypes::TPSAAtomTypes::
                       GetAllPossibleTPSAAtomTypes();
```

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

GetTPSAAtomTypesData

```
$AtomTypesDataMapRef = $TPSAAtomTypes->GetTPSAAtomTypesData();
$AtomTypesDataMapRef = AtomTypes::TPSAAtomTypes::GetTPSAAtomTypesData();
```

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

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

IsAtomTypesAssignmentSuccessful

```
$Status = $AtomTypes->IsAtomTypesAssignmentSuccessful();
```

Returns 1 or 0 based on whether atom types assignment was successfully performed. This method overrides the same method available in the base class AtomTypes.pm used to derived this class. It checks for successful atom type assignments for nitrogen and oxygen atoms with an optional check for phosphorous and sulfur atoms.

StringifyTPSAAtomTypes

```
$String = $TPSAAtomTypes->StringifyTPSAAtomTypes();
```

Returns a string containing information about *TPSAAtomTypes* object.

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

AtomTypes.pm, AtomicInvariantsAtomTypes.pm, DREIDINGAtomTypes.pm, EStateAtomTypes.pm, FunctionalClassAtomTypes.pm, MMFF94AtomTypes.pm, SLogPAtomTypes.pm, SYBYLAtomTypes.pm, UFFAtomTypes.pm

COPYRIGHT