NAME

MolecularVolumeDescriptors

SYNOPSIS

use MolecularDescriptors::MolecularVolumeDescriptors;

use MolecularDescriptors::MolecularVolumeDescriptors qw(:all);

DESCRIPTION

MolecularVolumeDescriptors class provides the following methods:

new, GenerateDescriptors, GetDescriptorNames, GetVDWAtomRadiiAndVolumesData, StringifyMolecularVolumeDescriptors

MolecularVolumeDescriptors is derived from MolecularDescriptors class which in turn is derived from ObjectProperty base class that provides methods not explicitly defined in MolecularVolumeDescriptors, MolecularDescriptors 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>();
```

van der Waals molecular volume [Ref 93] (A**3/molecule) of a molecule is calculated using atomic and bonds contributions along with adjustments for aromatic and non-aromatic rings using the following equation:

```
vdwMolecularVolume = SumOfAtomicVDWVolumeContributions
                   - 5.92 * NumOfBonds
                   - 14.7 * NumOfAromaticRings
                   - 3.8 * NumOfNonAromaticRings
```

van der Waals atomic volume for atoms is taken from data file VDWAtomRadiiAndVolumes.csv distributed with MayaChemTools. It contains van der Waals atom radii and atom and volumes data for 38 elements; Table 2 [Ref 93] contains data for only 15 elements. After converting valid van der Waals atom radius data from pm (picometer) to A (Angstrom) available under column name VanderWaalsRadius in PeriodicTableElementsData.csv data file, van der Waals atom volume is calculated using: 4/3 * PI * (Radius ** 3). For elements specified in Table 2 [Ref 93] - H, B, C, N, O, F, Si, P, S, Cl, As, Se, Br, Te, I - the van der Waals atom radii and calculated atom volumes match the values in the table.

METHODS

new

```
$NewMolecularVolumeDescriptors = new MolecularDescriptors::
                                 MolecularVolumeDescriptors(
                                 %NamesAndValues);
```

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

```
Molecule = ''
Type = 'MolecularVolume'
@DescriptorNames = ('MolecularVolume')
@DescriptorValues = ('None')
```

Examples:

```
$MolecularVolumeDescriptors = new MolecularDescriptors::
                              MolecularVolumeDescriptors();

$MolecularVolumeDescriptors->SetMolecule($Molecule);
$MolecularVolumeDescriptors->GenerateDescriptors();
print "MolecularVolumeDescriptors: $MolecularVolumeDescriptors\n";
```

GenerateDescriptors

```
$MolecularVolumeDescriptors->GenerateDescriptors();
```

Calculate van der Waals molecular volume descriptor for a molecule and returns *MolecularVolumeDescriptors*.

GetDescriptorNames

```
@DescriptorNames = $MolecularVolumeDescriptors->GetDescriptorNames();
@DescriptorNames = MolecularDescriptors::MolecularVolumeDescriptors::
                       GetDescriptorNames();
```

Returns all available descriptor names as an array.

GetVDWAtomRadiiAndVolumesData

```
$VDWVolumeDataMapRef = $MolecularVolumeDescriptors->
                           GetVDWAtomRadiiAndVolumesData();
$VDWVolumeDataMapRef = MolecularDescriptors::MolecularVolumeDescriptors::
                           GetVDWAtomRadiiAndVolumesData();
```

Returns a hash reference to van der Waals atom symbols corresponding to atom types and associated data loaded from VDWAtomRadiiAndVolumes.csv data file as a reference to hash with the following hash data format:

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

StringifyMolecularVolumeDescriptors

```
$String = $MolecularVolumeDescriptors->
                           StringifyMolecularVolumeDescriptors();
```

Returns a string containing information about *MolecularVolumeDescriptors* object.

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SEE ALSO

MolecularDescriptors.pm, MolecularDescriptorsGenerator.pm

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