NAME

AtomsCountDescriptors

SYNOPSIS

use MolecularDescriptors::AtomsCountDescriptors;

use MolecularDescriptors::AtomsCountDescriptors qw(:all);

DESCRIPTION

AtomsCountDescriptors class provides the following methods:

new, GenerateDescriptors, GetDescriptorNames, StringifyAtomsCountDescriptors

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

AtomsCountDescriptors class counts the number of atoms and heavy atoms in a molecule corresponding to total number of atom and non-hydrogen atoms respectively.

METHODS

new

```
$NewAtomsCountDescriptors = new MolecularDescriptors::
                            AtomsCountDescriptors(
                            %NamesAndValues);
```

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

```
Molecule = ''
Type = 'AtomsCount'

@DescriptorNames = ('Atoms', 'HeavyAtoms')
@DescriptorValues = ('None', 'None')
```

Examples:

```
$AtomsCountDescriptors = new AtomsCountDescriptors(
                            'Molecule' => $Molecule);

$AtomsCountDescriptors = new AtomsCountDescriptors();

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

GenerateDescriptors

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

Calculates number of atoms and heavy atoms in a molecule and returns *AtomsCountDescriptors*.

GetDescriptorNames

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

Returns all available descriptor names as an array.

StringifyAtomsCountDescriptors

```
$String = $AtomsCountDescriptors->StringifyAtomsCountDescriptors();
```

Returns a string containing information about *AtomsCountDescriptors* object.

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SEE ALSO

MolecularDescriptors.pm, MolecularDescriptorsGenerator.pm

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