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>();
```

Molecule = ''

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

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:

print "AtomsCountDescriptors: \$AtomsCountDescriptors\n";

GenerateDescriptors

```
{\tt \$AtomsCountDescriptors->GenerateDescriptors();}
```

\$AtomsCountDescriptors->SetMolecule(\$Molecule);
\$AtomsCountDescriptors->GenerateDescriptors();

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

GetDescriptorNames

Returns all available descriptor names as an array.

StringifyAtomsCountDescriptors

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

Returns a string containing information about AtomsCountDescriptors object.

AUTHOR

Manish Sud <msud@san.rr.com>

www.MayaChemTools.org Page 1

SEE ALSO

MolecularDescriptors.pm, MolecularDescriptorsGenerator.pm

COPYRIGHT

Copyright (C) 2017 Manish Sud. All rights reserved.

This file is part of MayaChemTools.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version.

www.MayaChemTools.org Page 2