

NAME

WeightAndMassDescriptors

SYNOPSIS

```
use MolecularDescriptors::WeightAndMassDescriptors;

use MolecularDescriptors::WeightAndMassDescriptors qw(:all);
```

DESCRIPTION

WeightAndMassDescriptors class provides the following methods:

new, GenerateDescriptors, GetDescriptorNames, StringifyWeightAndMassDescriptors

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

WeightAndMassDescriptors calculates molecular weight and exact mass descriptors using methods available in Molecule class.

METHODS

new

```
$NewWeightAndMassDescriptors = new MolecularDescriptors::
    WeightAndMassDescriptors(
        %NamesAndValues);
```

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

```
Molecule = ''
Type = 'WeightAndMass'
WeightPrecision = 2;
MassPrecision = 4;

@DescriptorNames = ('MolecularWeight', 'ExactMass')
@DescriptorValues = ('None', 'None')
```

Examples:

```
$WeightAndMassDescriptors = new MolecularDescriptors::
    WeightAndMassDescriptors(
        'Molecule' => $Molecule);

$WeightAndMassDescriptors = new MolecularDescriptors::
    WeightAndMassDescriptors();

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

GenerateDescriptors

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

Calculates molecular weight and exact mass of a molecule and returns *WeightAndMassDescriptors*.

GetDescriptorNames

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

Returns all available descriptor names as an array.

SetMassPrecision

```
$WeightAndMassDescriptors->SetMassPrecision($Precision);
```

Sets precision for calculated exact mass value and returns *WeightAndMassDescriptors*.

SetWeightPrecision

```
$WeightAndMassDescriptors->SetWeightPrecision($Precision);
```

Sets precision for calculated molecular weight value and returns *WeightAndMassDescriptors*.

StringifyWeightAndMassDescriptors

```
$String = $WeightAndMassDescriptors->StringifyWeightAndMassDescriptors();
```

Returns a string containing information about *WeightAndMassDescriptors* object.

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

MolecularDescriptors.pm, MolecularDescriptorsGenerator.pm

COPYRIGHT

Copyright (C) 2018 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.