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

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:
```

GenerateDescriptors

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

Calculates molecular weight and exact mass of a molecule and returns 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

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

Sets precision for calculated molecular weight value and returns WeightAndMassDescriptors.

Stringify Weight And Mass Descriptors

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

Returns a string containing information about WeightAndMassDescriptors object.

AUTHOR

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SEE ALSO

 $Molecular Descriptors.pm,\ Molecular Descriptors Generator.pm$

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