## NAME

MolecularDescriptors - MolecularDescriptors class

## SYNOPSIS

use MolecularDescriptors;

use MolecularDescriptors qw(:all);

## DESCRIPTION

MolecularDescriptors base class used to derive all other molecular descriptors classes provides the following methods:

new, AddDescriptorNames, AddDescriptorValues, GetDescriptorNames, GetDescriptorNamesAndValues, GetDescriptorValueByName, GetDescriptorValues, IsDescriptorsGenerationSuccessful, SetDescriptorNames, SetDescriptorValues, SetMolecule, SetType

MolecularDescriptors class is derived from ObjectProperty base class which provides methods not explicitly defined in Fingerprints 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>();
```

## METHODS

### new

```
$NewMolecularDescriptors = new MolecularDescriptors(%NamesAndValues);
```

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

```
Molecule = '';
Type = '';
```

### AddDescriptorNames

```
$MolecularDescriptors->AddDescriptorNames(@Name);
```

Adds specified descriptor *Names* to the list of available descriptor names and returns *MolecularDescriptors*.

### AddDescriptorValues

```
$MolecularDescriptors->AddDescriptorValues(@Values);
```

Adds specified descriptor *Values* to the list of calculated descriptor values and returns *MolecularDescriptors*.

### GetDescriptorNames

```
@Names = $MolecularDescriptors->GetDescriptorNames();
```

Returns an array containing all available descriptor names.

### GetDescriptorNamesAndValues

```
%NamesAndValuesReturn = $MolecularDescriptors->
                            GetDescriptorNamesAndValues();
```

Returns a hash containing all available descriptor names and calculated values.

### GetDescriptorValueByName

```
$Value = $MolecularDescriptors->
                            GetDescriptorValueByName($Name);
```

Returns calculated value for a specified descriptor name. A string None is returned for unknown descriptor names or for those descriptors whose values haven't been calculated.

### GetDescriptorValues

```
@Values = $MolecularDescriptors->GetDescriptorValues();
```

Returns an array containing calculated descriptor values for all available descriptors. Unless CalculateDescriptorsValues method has been successfully invoked on a *MolecularDescriptors* object, value of each descriptor corresponds to string None.

### IsDescriptorsGenerationSuccessful

```
$Status = $MolecularDescriptors->
                            IsDescriptorsGenerationSuccessful();
```

Returns 1 or 0 based on whether molecular descriptors generation was successful. For a successful molecular descriptors calculation, all available descriptors must have a values other than a string *None* which are set by CalculateDescriptorsValues method after successful completion of descriptors calculation.

SetDescriptorNames

```
$MolecularDescriptors->SetDescriptorNames(@Names);
```

Sets names of available descriptors to specified names and returns *MolecularDescriptors*.

SetDescriptorValues

```
$MolecularDescriptors->SetDescriptorValues(@Values);
```

Sets values of available descriptors to specified values and returns *MolecularDescriptors*.

SetMolecule

```
$MolecularDescriptors->SetMolecule($Molecule);
```

Sets molecule to use during calculation of molecular descriptors and returns *MolecularDescriptors*.

SetType

```
$MolecularDescriptors->SetType($Type);
```

Sets *Type* for *MolecularDescriptors* object and returns *MolecularDescriptors*.

## AUTHOR

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## SEE ALSO

MolecularDescriptorsGenerator.pm

## COPYRIGHT