NAME

RotatableBondsDescriptors

SYNOPSIS

use MolecularDescriptors::RotatableBondsDescriptors;

use MolecularDescriptors::RotatableBondsDescriptors qw(:all);

DESCRIPTION

RotatableBondsDescriptors class provides the following methods:

new, GenerateDescriptors, GetDescriptorNames, StringifyRotatableBondsDescriptors

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

A rotatable bond [Ref 92] is defined as any single bond which is not in a ring and involves only non-hydrogen
atoms. By default, the following types of single bonds are not considered rotatable bonds:

```
o Terminal bonds
o Bonds attached to triple bonds
o Amide C-N bonds
o Thioamide C-N bond bonds
o Sulfonamide S-N bonds
```

METHODS

new

```
$RotatableBondsDescriptors = new MolecularDescriptors::
                             RotatableBondsDescriptors(
                             %NamesAndValues);
```

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

```
Molecule = ''
Type = 'RotatableBonds'
IgnoreTerminalBonds = 1
IgnoreBondsToTripleBonds = 1
IgnoreAmideBonds = 1
IgnoreThioamideBonds = 1
IgnoreSulfonamideBonds = 1
@DescriptorNames = ('RotatableBonds')
@DescriptorValues = ('None')
```

Examples:

```
$RotatableBondsDescriptors = new MolecularDescriptors::
                             RotatableBondsDescriptors();

$RotatableBondsDescriptors = new MolecularDescriptors::
                             RotatableBondsDescriptors(
                             'IgnoreAmideBonds' => 0,
                             'IgnoreThioamideBonds' => 0,
                             'IgnoreSulfonamideBonds' => 0);

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

GenerateDescriptors

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

Calculates number of rotatable bonds descriptors in a molecule and returns *RotatableBondsDescriptors*.

GetDescriptorNames

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

Returns all available descriptor names as an array.

StringifyRotatableBondsDescriptors

```
$String = $RotatableBondsDescriptors->StringifyRotatableBondsDescriptors();
```

Returns a string containing information about *RotatableBondsDescriptors* object.

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SEE ALSO

MolecularDescriptors.pm, MolecularDescriptorsGenerator.pm

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