NAME

SLogPAndSMRDescriptors

SYNOPSIS

use MolecularDescriptors::SLogPAndSMRDescriptors;

use MolecularDescriptors::SLogPAndSMRDescriptors qw(:all);

DESCRIPTION

SLogPAndSMRDescriptors class provides the following methods:

new, GenerateDescriptors, GetDescriptorNames, StringifySLogPAndSMRDescriptors

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

After SLogP atom types [Ref 89] has been assigned to all atoms in a molecule using AtomTypes::SLogPAndSMR.pm module, SLogP (calculated logP) and SMR (calculated molar refractivity) values are calculated by adding up LogP and MR contributions of each atom type.

METHODS

new

```
$NewSLogPAndSMRDescriptors = new MolecularDescriptors::
                             SLogPAndSMRDescriptors(
                             %NamesAndValues);
```

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

```
Molecule = ''
Type = 'SLogPAndSMR'
@DescriptorNames = ('SLogP', 'SMR')
@DescriptorValues = ('None', 'None')
```

Examples:

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

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

GenerateDescriptors

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

Calculate SLogP and SMR values for a molecule and returns *SLogPAndSMRDescriptors*.

GetDescriptorNames

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

Returns all available descriptor names as an array.

StringifySLogPAndSMRDescriptors

```
$String = $SLogPAndSMRDescriptors->StringifySLogPAndSMRDescriptors();
```

Returns a string containing information about *SLogPAndSMRDescriptors* object.

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SEE ALSO

MolecularDescriptors.pm, MolecularDescriptorsGenerator.pm

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