NAME

AtomicDescriptors - AtomicDescriptors class

SYNOPSIS

use AtomicDescriptors::AtomicDescriptors;

use AtomicDescriptors::AtomicDescriptors qw(:all);

DESCRIPTION

AtomicDescriptors base class used to derive all other atomic descriptors classes provides the following methods:

new, GetDescriptorValue, GetDescriptorValues, IsDescriptorsGenerationSuccessful, SetDescriptorValue

AtomicDescriptors 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

```
$NewAtomicDescriptors = new AtomicDescriptors::
                            AtomicDescriptors(%NamesAndValues);
```

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

```
Molecule = '';
Type = '';
IgnoreHydrogens = 0;
```

GetDescriptorValue

```
$Value = $AtomicDescriptors->GetDescriptorValue($Atom);
```

Returns calculated atomic descriptor *Value* for specified *Atom*.

GetDescriptorValues

```
%Values = $AtomicDescriptors->GetDescriptorValues();
```

Returns calculated atomic descriptor values for all atoms as a hash with atom ID and atomic descriptor values as key/value pairs.

IsDescriptorsGenerationSuccessful

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

Returns 1 or 0 based on whether atomic desctiptors calculations was successful. For a successful atomic descriptors calculation, all atoms must have a value of other than a string *None*.

SetDescriptorValue

```
$AtomicDescriptors->SetDescriptorValue($Atom, $Value);
```

Sets specified atomic descriptor *Value* for *Atom* and returns *$AtomicDescriptors*.

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SEE ALSO

demo

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