

NAME

AtomicDescriptors - AtomicDescriptors class

SYNOPSIS

```
use AtomicDescriptors;

use 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(%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 descriptors 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*.

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

`demo`

COPYRIGHT

Copyright (C) 2004-2012 Manish Sud. All rights reserved.

This file is part of MayaChemTools.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version.