

# 1,2,4-Oxadiazole, 3,5-diphenyl-

<b>Other names:</b>	3,5-Diphenyl-1,2,4-oxadiazole
<b>Inchi:</b>	InChI=1S/C14H10N2O/c1-3-7-11(8-4-1)13-15-14(17-16-13)12-9-5-2-6-10-12/h1-10H
<b>InchiKey:</b>	VIZNDSYPXQJMCM-UHFFFAOYSA-N
<b>Formula:</b>	C14H10N2O
<b>SMILES:</b>	<chem>c1ccc(-c2noc(-c3ccccc3)n2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	222.24
<b>CAS:</b>	888-71-1

## Physical Properties

Property code	Value	Unit	Source
chs	-7145.00 ± 11.00	kJ/mol	NIST Webbook
ie	9.20 ± 0.10	eV	NIST Webbook
log10ws	-9.94		Crippen Method
logp	3.404		Crippen Method
mcvol	166.970	ml/mol	McGowan Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	483.20	K	2.30	NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C888711&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C888711&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>tbrp:</b>	Boiling point at reduced pressure

Latest version available from:

<https://www.cheméo.com/cid/70-280-3/1-2-4-Oxadiazole-3-5-diphenyl.pdf>

Generated by Cheméo on 2024-05-01 23:01:11.795859778 +0000 UTC m=+16893720.716437094.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.