

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

<b>Other names:</b>	2,5-Diphenyloxadiazole 2,5-Diphenyl-1,3,4-oxadiazole PPD PPD (Scintillator)
<b>Inchi:</b>	InChI=1S/C14H10N2O/c1-3-7-11(8-4-1)13-15-16-14(17-13)12-9-5-2-6-10-12/h1-10H
<b>InchiKey:</b>	DCJKUXYSYJBBRD-UHFFFAOYSA-N
<b>Formula:</b>	C14H10N2O
<b>SMILES:</b>	<chem>c1ccc(-c2nnc(-c3ccccc3)o2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	222.24
<b>CAS:</b>	725-12-2

## Physical Properties

Property code	Value	Unit	Source
chs	-7014.00 ± 4.00	kJ/mol	NIST Webbook
chs	-7103.60 ± 8.40	kJ/mol	NIST Webbook
hfs	75.70	kJ/mol	NIST Webbook
ie	8.90 ± 0.30	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	504.20	K	1.70	NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C725122&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C725122&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>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<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

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