

# Isoxazole, 3,5-diphenyl-

<b>Other names:</b>	3,5-Diphenyl-1,2-oxazole 3,5-Diphenylisoxazole
<b>Inchi:</b>	InChI=1S/C15H11NO/c1-3-7-12(8-4-1)14-11-15(17-16-14)13-9-5-2-6-10-13/h1-11H
<b>InchiKey:</b>	HECRDSFKLUVCAI-UHFFFAOYSA-N
<b>Formula:</b>	C15H11NO
<b>SMILES:</b>	<chem>c1ccc(-c2cc(-c3ccccc3)on2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	221.25
<b>CAS:</b>	2039-49-8

## Physical Properties

Property code	Value	Unit	Source
chs	-7619.50 ± 7.50	kJ/mol	NIST Webbook
log10ws	-10.18		Crippen Method
logp	4.009		Crippen Method
mcvol	171.080	ml/mol	McGowan Method

## 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=C2039498&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2039498&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>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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