Isoxazole, 3,5-diphenyl-

Other names:	3,5-Diphenyl-1,2-oxazole
	3,5-Diphenylisoxazole
Inchi:	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
InchiKey:	HECRDSFKLUVCAY-UHFFFAOYSA-N
Formula:	C15H11NO
SMILES:	c1ccc(-c2cc(-c3ccccc3)on2)cc1
Mol. weight [g/mol]:	221.25
CAS:	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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2039498&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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