

1H-Isoindol-1-one, 2,3-dihydro-3-imino-2-phenyl-

Inchi:	InChI=1S/C14H10N2O/c15-13-11-8-4-5-9-12(11)14(17)16(13)10-6-2-1-3-7-10/h1-9,15H
InchiKey:	QEJRHIHNPZXIDK-UHFFFAOYSA-N
Formula:	C14H10N2O
SMILES:	N=C1c2ccccc2C(=O)N1c1ccccc1
Mol. weight [g/mol]:	222.24
CAS:	34446-14-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.72		Crippen Method
logp	2.672		Crippen Method
mcvol	166.970	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34446145&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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