

3,7-Diazaadamantan-9-one, 1,5-diphenyl-

Other names:	1,5-Diphenyl-3,7-diazaadamantan-9-one 1,3-Diazatricyclo[3.3.1.1
Inchi:	InChI=1S/C20H20N2O/c23-18-19(16-7-3-1-4-8-16)11-21-13-20(18,14-22(12-19)15-21)1
InchiKey:	XBSYMZDMKDGCCA-UHFFFAOYSA-N
Formula:	C20H20N2O
SMILES:	O=C1C2(c3ccccc3)CN3CN(C2)CC1(c1ccccc1)C3
Mol. weight [g/mol]:	304.39
CAS:	19066-35-4

Physical Properties

Property code	Value	Unit	Source
ie	7.87 ± 0.03	eV	NIST Webbook
log10ws	-2.35		Crippen Method
logp	2.034		Crippen Method
mcvol	234.090	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19066354&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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