# 5,7-Diphenyl-1,3-diazaadamantan-6-one

**Other names:** 1,5-Diphenyl-3,7-diazaadmantan-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)17
**InchiKey:** XBSYMZDMKDGCCA-UHFFFAOYSA-N
**Formula:** C20H20N2O
**SMILES:** O=C1C2(c3ccccc3)CN3CN(C2)CC1(c1ccccc1)C3
**Mol. weight [g/mol]:** 304.39

## Physical Properties

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

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C19066354&Units=SI
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**

## Legend

**ie:** Ionization energy
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume