# Ethanone,1-(4-chlorophenyl)-2-diazo-

**Inchi:** InChI=1S/C8H5ClN2O/c9-7-3-1-6(2-4-7)8(12)5-11-10/h1-5H
**InchiKey:** ZDKVKKYKIPGOBL-UHFFFAOYSA-N
**Formula:** C8H5ClN2O
**SMILES:** [N-]=[N+]=CC(=O)c1ccc(Cl)cc1
**Mol. weight [g/mol]:** 180.59
**CAS:** 3282-33-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| ie | 9.02 ± 0.05 | eV | NIST Webbook |
| log10ws | -4.45 | | Crippen Method |
| logp | 1.823 | | Crippen Method |
| mcvol | 124.990 | 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=C3282335&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

## 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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