# 3-Phenyl-4H-1,2,4-oxadiazol-5-one

**Other names:** 3-phenyl-1,2,4-oxadiazol-5(4H)-one
**Inchi:** InChI=1S/C8H6N2O2/c11-8-9-7(10-12-8)6-4-2-1-3-5-6/h1-5H,(H,9,10,11)
**InchiKey:** LMBDRBXGTCUBIH-UHFFFAOYSA-N
**Formula:** C8H6N2O2
**SMILES:** O=c1[nH]c(-c2ccccc2)no1
**Mol. weight [g/mol]:** 162.15

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -3896.10 ± 5.90 | kJ/mol | NIST Webbook |
| logp | 0.548 | | Crippen Method |
| mcvol | 112.060 | ml/mol | McGowan Method |

## Sources

**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C1456220&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

## Legend

**chs:** Standard solid enthalpy of combustion
**logp:** Octanol/Water partition coefficient
**mcvol:** McGowan's characteristic volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.