

# 3-Cyclobutene-1,2-dione, 3-phenyl-

**Other names:** Cyclobutenedione, phenyl-  
Phenylcyclobutenedione  
3-phenyl-3-cyclobutene-1,2-dione

**Inchi:** InChI=1S/C10H6O2/c11-9-6-8(10(9)12)7-4-2-1-3-5-7/h1-6H

**InchiKey:** KLGVPAWHYZDGCX-UHFFFAOYSA-N

**Formula:** C10H6O2

**SMILES:** O=c1cc(-c2cccc2)c1=O

**Mol. weight [g/mol]:** 158.15

**CAS:** 3947-97-5

## Physical Properties

Property code	Value	Unit	Source
chs	-4708.46 ± 0.71	kJ/mol	NIST Webbook
chs	-4708.46 ± 0.71	kJ/mol	NIST Webbook
hfs	-84.18	kJ/mol	NIST Webbook
hsub	54.39 ± 0.42	kJ/mol	NIST Webbook
hsub	54.40	kJ/mol	NIST Webbook
log10ws	-1.75		Crippen Method
logp	0.950		Crippen Method
mcvol	115.980	ml/mol	McGowan Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C3947975&Units=SI>

## Legend

**chs:** Standard solid enthalpy of combustion

**hfs:** Solid phase enthalpy of formation at standard conditions  
**hsub:** Enthalpy of sublimation at standard conditions  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

Latest version available from:

<https://www.cheméo.com/cid/77-046-6/3-Cyclobutene-1-2-dione-3-phenyl.pdf>

Generated by Cheméo on 2024-04-25 17:29:43.88264353 +0000 UTC m=+16355432.803220846.

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