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(-c2ccccc2)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/ci990307l
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=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