3-Cyclobutene-1,2-dione

Other names: Diketocyclobutene
Inchi: InChI=1S/C4H2O2/c5-3-1-2-4(3)6/h1-2H
InchiKey: RGBVWCQARBEPPW-UHFFFAOYSA-N
Formula: C4H2O2
SMILES: O=c1ccc1=O
Mol. weight [g/mol]: 82.06
CAS: 32936-74-6

Physical Properties

Property code	Value	Unit	Source
ie	9.79	eV	NIST Webbook
log10ws	0.85		Crippen Method
logp	-0.717		Crippen Method
mcvol	55.200	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C32936746&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume