3-Cyclobutene-1,2-dione, 3,4-dimethyl-

Inchi: InChI=1S/C6H6O2/c1-3-4(2)6(8)5(3)7/h1-2H3
InchiKey: XSPNWUVAVYEPBO-UHFFFAOYSA-N
Formula: C6H6O2
SMILES: Cc1c(C)c(=O)c1=O
Mol. weight [g/mol]: 110.11
CAS: 1121-15-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.10		Crippen Method
logp	-0.101		Crippen Method
mcvol	83.380	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1121159&Units=SI
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

Legend

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