

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/ci9903071
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

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