

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

Other names:	Squaric acid Cyclobutenedione, dihydroxy- Quadratic acid 1,2-Dihydroxycyclobutene-3,4-dione 1,2-Diketo-3,4-dihydroxycyclobutene 3,4-Dihydroxy-3-cyclobutene-1,2-dione 1,2-Dihydroxy cyclobutenedione 1,2-Dihydroxy-3,4-cyclobutenedione Cyclobutene-1,2-dione, 3,4-dihydroxy- 3,4-Dihydroxy-cyclobutene-1,2-dione NSC 125692
Inchi:	InChI=1S/C4H2O4/c5-1-2(6)4(8)3(1)7/h5-6H
InchiKey:	PWEBUXCTKOWPCW-UHFFFAOYSA-N
Formula:	C4H2O4
SMILES:	O=c1c(O)c(O)c1=O
Mol. weight [g/mol]:	114.06
CAS:	2892-51-5

Physical Properties

Property code	Value	Unit	Source
log10ws	1.76		Crippen Method
logp	-1.306		Crippen Method
mcvol	66.940	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2892515&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

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