

Diketocyclobutene

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

Physical Properties

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

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C32936746&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/72-889-6/Diketocyclobutene.pdf>

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