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

Physical Properties

Property code	Value	Unit	Source
af	0.4783		Cheméo Relay (1.0)
hf	-206.21	kJ/mol	Cheméo Relay (1.0)
hvap	56.82	kJ/mol	Cheméo Relay (1.0)
ie	9.10	eV	NIST Webbook
ie	9.06	eV	NIST Webbook
log10ws	-0.84		Cheméo Relay (1.0)
logp	-0.101		Crippen Method
mcvol	83.380	ml/mol	McGowan Method
pc	4075.21	kPa	Cheméo Relay (1.0, beta)
tb	461.50	K	Cheméo Relay (1.0)
tc	674.76	K	Cheméo Relay (1.0)
tf	438.36	K	Cheméo Relay (1.0)
vc	0.316	m3/kmol	Cheméo Relay (1.0)

Sources

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1121159&Units=SI

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume