

# 1,3-Cyclohexanedione, 4,4-dimethyl-

Inchi:	InChI=1S/C8H12O2/c1-8(2)4-3-6(9)5-7(8)10/h3-5H2,1-2H3
InchiKey:	PLGPBTCNKJQJHQ-UHFFFAOYSA-N
Formula:	C8H12O2
SMILES:	CC1(C)CCC(=O)CC1=O
Mol. weight [g/mol]:	140.18
CAS:	562-46-9

## Physical Properties

Property code	Value	Unit	Source
chs	-4363.50 ± 1.30	kJ/mol	NIST Webbook
gf	-209.74	kJ/mol	Joback Method
hf	-400.40 ± 2.70	kJ/mol	NIST Webbook
hfs	-499.60 ± 1.70	kJ/mol	NIST Webbook
hfus	1.03	kJ/mol	Joback Method
hsub	99.20 ± 2.10	kJ/mol	NIST Webbook
hsub	99.20 ± 2.10	kJ/mol	NIST Webbook
hvap	41.17	kJ/mol	Joback Method
log10ws	-1.38		Crippen Method
logp	1.335		Crippen Method
mcvol	115.860	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
tb	537.87	K	Joback Method
tc	785.42	K	Joback Method
tf	347.64	K	Joback Method
vc	0.428	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.77	J/mol×K	537.87	Joback Method
cpg	292.13	J/mol×K	579.13	Joback Method
cpg	307.63	J/mol×K	620.39	Joback Method
cpg	322.36	J/mol×K	661.64	Joback Method
cpg	336.38	J/mol×K	702.90	Joback Method

cpg	349.76	J/mol×K	744.16	Joback Method
cpg	362.57	J/mol×K	785.42	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.20	K	0.90	NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C562469&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C562469&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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