

1,3-CYCLOPENTANEDIONE

Other names:	1,3-Cyclopentadione cyclopentane-1,3-dione
Inchi:	InChI=1S/C5H6O2/c6-4-1-2-5(7)3-4/h1-3H2
InchiKey:	LOGSONSNCYTHPS-UHFFFAOYSA-N
Formula:	C5H6O2
SMILES:	O=C1CCC(=O)C1
Mol. weight [g/mol]:	98.10

Physical Properties

Property code	Value	Unit	Source
af	0.4131		Cheméo Relay (1.0)
gf	-209.70	kJ/mol	Joback Method
hf	-278.64	kJ/mol	Cheméo Relay (1.0)
hfus	0.59	kJ/mol	Joback Method
hvap	43.88	kJ/mol	Cheméo Relay (1.0)
ie	9.46 ± 0.05	eV	NIST Webbook
ie	9.53	eV	NIST Webbook
log10ws	0.11		Cheméo Relay (1.0)
logp	0.308		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
pc	4994.44	kPa	Joback Method
tb	452.91	K	Cheméo Relay (1.0)
tc	665.79	K	Cheméo Relay (1.0)
tf	423.00 ± 3.00	K	NIST Webbook
vc	0.253	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.97	J/mol×K	469.39	Joback Method
cpg	158.12	J/mol×K	509.65	Joback Method
cpg	168.92	J/mol×K	549.91	Joback Method
cpg	179.31	J/mol×K	590.17	Joback Method
cpg	189.25	J/mol×K	630.43	Joback Method

cpg	198.71	J/mol×K	670.69	Joback Method
cpg	207.63	J/mol×K	710.95	Joback Method

Sources

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=C3859414&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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

Latest version available from:

<https://www.chemeo.com/cid/25-311-8/1-3-CYCLOPENTANEDIONE.pdf>

Generated by Cheméo on 2026-07-21 20:55:08.515871647 +0000 UTC m=+178404.357757037.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.