1,2-CYCLOPENTANEDIONE

Inchi: InChI=1S/C5H6O2/c6-4-2-1-3-5(4)7/h1-3H2
InchiKey: CIISBNCSMVCNIP-UHFFFAOYSA-N
Formula: C5H6O2
SMILES: O=C1CCCC1=O
Mol. weight [g/mol]: 98.10

Physical Properties

Property code	Value	Unit	Source
af	0.4194		Cheméo Relay (1.0)
gf	-209.70	kJ/mol	Joback Method
hf	-261.71	kJ/mol	Cheméo Relay (1.0)
hfus	0.59	kJ/mol	Joback Method
hvap	52.13	kJ/mol	Cheméo Relay (1.0)
ie	9.54	eV	Cheméo Relay (1.0)
log10ws	-0.25		Cheméo Relay (1.0)
logp	0.308		Crippen Method
mcvol	73.590	ml/mol	McGowan Method
pc	4994.44	kPa	Joback Method
tb	452.26	K	Cheméo Relay (1.0)
tc	703.20	K	Cheméo Relay (1.0)
tf	366.67	K	Cheméo Relay (1.0)
vc	0.261	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

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
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=C3008400&Units=SI

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