1,4-Cyclohexanedione

Other names:	Tetrahydroquinone
	1,4-Dioxocyclohexane
	Cyclohexane-1,4-dione
Inchi:	InChI=1S/C6H8O2/c7-5-1-2-6(8)4-3-5/h1-4H2
InchiKey:	DCZFGQYXRKMVFG-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	O=C1CCC(=O)CC1
Mol. weight [g/mol]:	112.13
CAS:	637-88-7

Physical Properties

Property code	Value	Unit	Source
affp	812.50	kJ/mol	NIST Webbook
basg	782.70	kJ/mol	NIST Webbook
chs	-3096.80 ± 0.60	kJ/mol	NIST Webbook
gf	-213.38	kJ/mol	Joback Method
hf	-332.60 ± 1.20	kJ/mol	NIST Webbook
hfs	-407.60 ± 1.00	kJ/mol	NIST Webbook
hfus	1.08	kJ/mol	Joback Method
hsub	75.00 ± 1.00	kJ/mol	NIST Webbook
hsub	75.00 ± 1.00	kJ/mol	NIST Webbook
hsub	84.20	kJ/mol	NIST Webbook
hvap	38.18	kJ/mol	Joback Method
ie	9.65	eV	NIST Webbook
ie	9.85	eV	NIST Webbook
log10ws	-0.79		Crippen Method
logp	0.699		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
ripol	1975.00		NIST Webbook
ripol	1975.00		NIST Webbook
tb	496.54	K	Joback Method
tc	743.28	K	Joback Method
tf	350.00 ± 1.00	K	NIST Webbook
tf	351.15 ± 1.00	K	NIST Webbook
tt	351.60 ± 0.20	K	NIST Webbook
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.49	J/mol×K	702.15	Joback Method
cpg	238.21	J/mol×K	661.03	Joback Method
cpg	260.02	J/mol×K	743.28	Joback Method
cpg	186.73	J/mol×K	496.54	Joback Method
cpg	200.45	J/mol×K	537.66	Joback Method
cpg	213.64	J/mol×K	578.79	Joback Method
cpg	226.25	J/mol×K	619.91	Joback Method
cps	161.40	J/mol×K	300.00	NIST Webbook
hfust	6.15	kJ/mol	322.20	NIST Webbook
hfust	10.04	kJ/mol	348.20	NIST Webbook
hfust	0.96	kJ/mol	339.20	NIST Webbook
hfust	11.26	kJ/mol	351.50	NIST Webbook
hfust	10.04	kJ/mol	348.20	NIST Webbook
hsubt	84.40	kJ/mol	289.00	NIST Webbook
hsubt	75.00	kJ/mol	298.15	NIST Webbook
sfust	28.84	J/mol×K	348.20	NIST Webbook
sfust	2.83	J/mol×K	339.20	NIST Webbook
sfust	19.09	J/mol×K	322.20	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C637887&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

affp: Proton affinity
basg: Gas basicity
chs: Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume