Cyclohexane-1,4-dione

Other names: 1,4-Dioxocyclohexane
1,4-cyclohexadione
1,4-cyclohexanedione
Tetrahydroquinone
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

Physical Properties

Property code	Value	Unit	Source
af	0.4307		Cheméo Relay (1.0)
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	84.20	kJ/mol	NIST Webbook
hsub	75.00 ± 1.00	kJ/mol	NIST Webbook
hsub	75.00 ± 1.00	kJ/mol	NIST Webbook
hvap	55.81	kJ/mol	Cheméo Relay (1.0)
ie	9.85	eV	NIST Webbook
ie	9.65	eV	NIST Webbook
log10ws	0.07		Cheméo Relay (1.0)
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	472.58	K	Cheméo Relay (1.0)
tc	682.49	K	Cheméo Relay (1.0)
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	0.298	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.73	J/mol×K	496.54	Joback Method
cpg	260.02	J/mol×K	743.28	Joback Method
cpg	249.49	J/mol×K	702.15	Joback Method
cpg	238.21	J/mol×K	661.03	Joback Method
cpg	226.25	J/mol×K	619.91	Joback Method
cpg	213.64	J/mol×K	578.79	Joback Method
cpg	200.45	J/mol×K	537.66	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	10.04	kJ/mol	348.20	NIST Webbook
hfust	11.26	kJ/mol	351.50	NIST Webbook
hsubt	75.00	kJ/mol	298.15	NIST Webbook
hsubt	84.40	kJ/mol	289.00	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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Partial molar volumes of organic solutes in water. XXIII. Cyclic ketones at T = (298 to 573) K and pressures up to 30 MPa : https://www.doi.org/10.1016/j.jct.2011.02.010

Partial Molar Volumes of Cyclic Ketones at Infinite Dilution in Water at Temperatures T = (278 to 373) K and Low Pressure : https://www.doi.org/10.1021/je100547a

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C637887&Units=SI

Legend

af:	Acentric Factor
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