1,3-Cyclohexanedione

Other names:	Dihydroresorcinol
	Cyclohexane-1,3-dione
	Hydroresorcinol
	Resorcinol, dihydro-
	1,3-Benzenediol, dihydro-
	1,3-Cyclohexandione
Inchi:	InChI=1S/C6H8O2/c7-5-2-1-3-6(8)4-5/h1-4H2
InchiKey:	HJSLFCCWAKVHIW-UHFFFAOYSA-N
Formula:	C6H8O2
SMILES:	O=C1CCCC(=O)C1
Mol. weight [g/mol]:	112.13
CAS:	504-02-9

Physical Properties

Property code	Value	Unit	Source
affp	881.20	kJ/mol	NIST Webbook
basg	849.40	kJ/mol	NIST Webbook
chs	-3079.00 ± 0.80	kJ/mol	NIST Webbook
gf	-213.38	kJ/mol	Joback Method
hf	-335.60 ± 1.60	kJ/mol	NIST Webbook
hfs	-425.40 ± 1.10	kJ/mol	NIST Webbook
hfus	1.08	kJ/mol	Joback Method
hsub	89.80 ± 1.10	kJ/mol	NIST Webbook
hsub	89.80 ± 1.10	kJ/mol	NIST Webbook
hvap	38.18	kJ/mol	Joback Method
ie	9.60	eV	NIST Webbook
ie	9.52 ± 0.05	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
tb	496.54	K	Joback Method
tc	743.28	K	Joback Method
tf	378.40 ± 2.00	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	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
cpg	238.21	J/mol×K	661.03	Joback Method
cpg	260.02	J/mol×K	743.28	Joback Method
hsubt	89.80	kJ/mol	298.15	NIST Webbook

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C504029&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
chs: Standard solid enthalpy of combustion
cpg: Ideal gas 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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume