1,2-Cyclohexanedione

Other names: 1,2-Dioxocyclohexane
Cyclohexane-1,2-dione
1,2-Cyclohexadione
c-hexane-1,2-dione
Inchi: InChI=1S/C6H8O2/c7-5-3-1-2-4-6(5)8/h1-4H2
InchiKey: OILAIQUEIWYQPH-UHFFFAOYSA-N
Formula: C6H8O2
SMILES: O=C1CCCCC1=O
Mol. weight [g/mol]: 112.13
CAS: 765-87-7

Physical Properties

Property code	Value	Unit	Source
affp	849.60	kJ/mol	NIST Webbook
basg	818.90	kJ/mol	NIST Webbook
gf	-213.38	kJ/mol	Joback Method
hf	-367.91	kJ/mol	Joback Method
hfus	1.08	kJ/mol	Joback Method
hvap	38.18	kJ/mol	Joback Method
log10ws	-0.79		Crippen Method
logp	0.699		Crippen Method
mcvol	87.680	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
ripol	1668.00		NIST Webbook
tb	467.20	K	NIST Webbook
tc	743.28	K	Joback Method
tf	305.44	K	Joback Method
vc	0.320	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	249.49	J/mol×K	702.15	Joback Method
cpg	260.02	J/mol×K	743.28	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C765877&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

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

Legend

affp: Proton affinity

basg: Gas basicity

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

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

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume