1,4-Cyclohex-2-enedione

Other names: 2-cyclohexene-1,4-dione
Inchi: InChI=1S/C6H6O2/c7-5-1-2-6(8)4-3-5/h1-2H,3-4H2
InchiKey: GPMMYQITJVUZAT-UHFFFAOYSA-N
Formula: C6H6O2
SMILES: O=C1C=CC(=O)CC1
Mol. weight [g/mol]: 110.11
CAS: 4505-38-8

Physical Properties

Property code	Value	Unit	Source
gf	-183.42	kJ/mol	Joback Method
hf	-310.13	kJ/mol	Joback Method
hfus	2.30	kJ/mol	Joback Method
hvap	38.47	kJ/mol	Joback Method
ie	9.77	eV	NIST Webbook
log10ws	-0.64		Crippen Method
logp	0.475		Crippen Method
mcvol	83.380	ml/mol	McGowan Method
pc	4756.24	kPa	Joback Method
rinpol	1032.00		NIST Webbook
rinpol	1024.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1044.00		NIST Webbook
tb	495.70	K	Joback Method
tc	745.13	K	Joback Method
tf	306.20	K	Joback Method
vc	0.305	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.10	J/mol×K	495.70	Joback Method
cpg	182.34	J/mol×K	537.27	Joback Method
cpg	194.10	J/mol×K	578.84	Joback Method

cpg	205.34	J/mol×K	620.42	Joback Method
cpg	215.99	J/mol×K	661.99	Joback Method
cpg	226.00	J/mol×K	703.56	Joback Method
cpg	235.32	J/mol×K	745.13	Joback Method

Sources

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=C4505388&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume