2,4-Cyclohexadien-1-one,6-methylene-

Inchi: InChI=1S/C7H6O/c1-6-4-2-3-5-7(6)8/h2-5H,1H2
InchiKey: NSDWWGAIPUNJAX-UHFFFAOYSA-N
Formula: C7H6O
SMILES: C=C1C=CC=CC1=O
Mol. weight [g/mol]: 106.12
CAS: 27890-67-1

Physical Properties

Property code	Value	Unit	Source
gf	30.63	kJ/mol	Joback Method
hf	-51.05	kJ/mol	Joback Method
hfus	5.45	kJ/mol	Joback Method
hvap	36.90	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
log10ws	-1.49		Crippen Method
logp	1.238		Crippen Method
mcvol	87.300	ml/mol	McGowan Method
pc	4294.29	kPa	Joback Method
tb	449.08	K	Joback Method
tc	680.19	K	Joback Method
tf	263.69	K	Joback Method
vc	0.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	159.01	J/mol×K	449.08	Joback Method
cpg	169.82	J/mol×K	487.60	Joback Method
cpg	180.14	J/mol×K	526.12	Joback Method
cpg	189.95	J/mol×K	564.63	Joback Method
cpg	199.26	J/mol×K	603.15	Joback Method
cpg	208.05	J/mol×K	641.67	Joback Method
cpg	216.31	J/mol×K	680.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C27890671&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume