2,5-Cyclohexadienone

Inchi: InChI=1S/C6H6O/c7-6-4-2-1-3-5-6/h2-5H,1H2
InchiKey: WGHKKEJHRMUKDK-UHFFFAOYSA-N
Formula: C6H6O
SMILES: O=C1C=CCC=C1
Mol. weight [g/mol]: 94.11
CAS: 5664-33-5

Physical Properties

Property code	Value	Unit	Source
gf	-30.87	kJ/mol	Joback Method
hf	-50.00 ± 10.00	kJ/mol	NIST Webbook
hfus	4.01	kJ/mol	Joback Method
hvap	34.52	kJ/mol	Joback Method
log10ws	-1.22		Crippen Method
logp	1.072		Crippen Method
mcvol	77.510	ml/mol	McGowan Method
pc	4762.81	kPa	Joback Method
tb	427.04	K	Joback Method
tc	659.38	K	Joback Method
tf	238.74	K	Joback Method
vc	0.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.24	J/mol×K	427.04	Joback Method
cpg	146.34	J/mol×K	465.76	Joback Method
cpg	156.91	J/mol×K	504.49	Joback Method
cpg	166.94	J/mol×K	543.21	Joback Method
cpg	176.43	J/mol×K	581.93	Joback Method
cpg	185.38	J/mol×K	620.66	Joback Method
cpg	193.78	J/mol×K	659.38	Joback Method

Sources

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=C5664335&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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