2,5-Cyclohexadien-1-one, 4-(4-oxo-2,5-cyclohexadien-1-ylidene)-

Other names: [Bi-2,5-cyclohexadien-1-ylidene]-4,4'-dione
Diphenoquinone
4,4'-Diphenoquinone

Inchi: InChI=1S/C12H8O2/c13-11-5-1-9(2-6-11)10-3-7-12(14)8-4-10/h1-8H

InchiKey: DDTHMESPCBONDT-UHFFFAOYSA-N

Formula: C12H8O2

SMILES: O=C1C=CC(=C2C=CC(=O)C=C2)C=C1

Mol. weight [g/mol]: 184.19

CAS: 494-72-4

Physical Properties

Property code	Value	Unit	Source
gf	-0.16	kJ/mol	Joback Method
hf	-151.13	kJ/mol	Joback Method
hfus	12.72	kJ/mol	Joback Method
hvap	55.06	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	1.673		Crippen Method
mcvol	139.860	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	663.80	K	Joback Method
tc	939.01	K	Joback Method
tf	413.52	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.34	J/mol×K	663.80	Joback Method
cpg	363.99	J/mol×K	709.67	Joback Method
cpg	378.31	J/mol×K	755.54	Joback Method
cpg	391.26	J/mol×K	801.41	Joback Method
cpg	402.82	J/mol×K	847.27	Joback Method
cpg	412.96	J/mol×K	893.14	Joback Method

cpg	421.66	J/mol×K	939.01	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=C494724&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
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