2,5-Cyclohexadiene-1,4-dione, 2-phenyl-

Other names:	p-Benzoquinone, 2-phenyl-
	Phenyl-p-benzoquinone
	Phenyl-1,4-benzoquinone
	Phenylquinone
	2-Phenyl-p-benzoquinone
	2-Phenyl-1,4-benzoquinone
	2-Phenylbenzoquinone
	Phenylbenzoquinone
	p-Benzoquinone, phenyl-
	2-Phenylquinone
	NSC 2806
	2-Phenylbenzo-1,4-quinone
Inchi:	InChI=1S/C12H8O2/c13-10-6-7-12(14)11(8-10)9-4-2-1-3-5-9/h1-8H
InchiKey:	RLQZIECDMISZHS-UHFFFAOYSA-N
Formula:	C12H8O2
SMILES:	O=C1C=CC(=O)C(c2ccccc2)=C1
Mol. weight [g/mol]:	184.19
CAS:	363-03-1

Physical Properties

Property code	Value	Unit	Source
ea	2.04 ± 0.06	eV	NIST Webbook
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	-2.28		Crippen Method
logp	1.778		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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C363031&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

Legend

cpg: Ideal gas heat capacity
ea: Electron affinity
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