p-Benzoquinone

Other names:	1,4-Benzoquine
	1,4-Benzoquinone
	1,4-Cyclohexadiene dioxide
	1,4-Cyclohexadienedione
	1,4-Diossibenzene
	1,4-Dioxy-benzol
	2,5-Cyclohexadiene-1,4-dione
	Benzo-chinon
	Benzoquinone
	Chinon
	Chinone
	Cyclohexadienedione
	NCI-C55845
	NSC 36324
	Quinone
	Rcra waste number U197
	Steara PBQ
	UN 2587
	USAF P-220
	p-Chinon
	p-Quinone
Inchi:	InChI=1S/C6H4O2/c7-5-1-2-6(8)4-3-5/h1-4H
InchiKey:	AZQWKYJCGOJGHM-UHFFFAOYSA-N
Formula:	C6H4O2
SMILES:	O=C1C=CC(=O)C=C1
Mol. weight [g/mol]:	108.09
CAS:	106-51-4

Physical Properties

Property code	Value	Unit	Source
affp	799.10	kJ/mol	NIST Webbook
basg	769.30	kJ/mol	NIST Webbook
chg	-2810.00 ± 4.00	kJ/mol	NIST Webbook
chs	-2725.80	kJ/mol	NIST Webbook
chs	-2745.90 ± 0.42	kJ/mol	NIST Webbook
chs	-2748.20	kJ/mol	NIST Webbook

chs	-2748.30	kJ/mol	NIST Webbook
chs	-2753.00	kJ/mol	NIST Webbook
ea	1.85 ± 0.01	eV	NIST Webbook
ea	1.99 ± 0.05	eV	NIST Webbook
ea	1.93 ± 0.05	eV	NIST Webbook
ea	1.91 ± 0.10	eV	NIST Webbook
ea	1.86 ± 0.01	eV	NIST Webbook
ea	1.89 ± 0.30	eV	NIST Webbook
ea	1.37 ± 0.08	eV	NIST Webbook
gf	-153.46	kJ/mol	Joback Method
hf	-252.35	kJ/mol	Joback Method
hfs	-184.50	kJ/mol	NIST Webbook
hfs	-186.80 ± 0.71	kJ/mol	NIST Webbook
hfs	-184.50 ± 0.63	kJ/mol	NIST Webbook
hfus	18.40	kJ/mol	Thermochemistry of benzoquinones
hsub	62.80	kJ/mol	NIST Webbook
hsub	62.76	kJ/mol	NIST Webbook
hsub	66.70 ± 1.60	kJ/mol	NIST Webbook
hvap	38.77	kJ/mol	Joback Method
ie	9.70	eV	NIST Webbook
ie	9.67 ± 0.02	eV	NIST Webbook
ie	9.95	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	9.96 ± 0.01	eV	NIST Webbook
ie	9.96 ± 0.01	eV	NIST Webbook
ie	10.03	eV	NIST Webbook
ie	10.01	eV	NIST Webbook
ie	10.11	eV	NIST Webbook
ie	10.00 ± 0.10	eV	NIST Webbook
ie	9.99 ± 0.05	eV	NIST Webbook
log10ws	-0.72		Aqueous Solubility Prediction Method
logp	0.251		Crippen Method
mcvol	79.080	ml/mol	McGowan Method
pc	5001.51	kPa	Joback Method
rinpol	912.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	143.19		NIST Webbook
rinpol	888.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	919.00		NIST Webbook
rinpol	147.33		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1579.00		NIST Webbook

ripol	1570.00		NIST Webbook
ripol	1562.00		NIST Webbook
tb	494.86	K	Joback Method
tc	747.03	K	Joback Method
tf	386.00 ± 0.30	K	NIST Webbook
tf	387.57	K	Aqueous Solubility Prediction Method
vc	0.291	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.43	J/mol×K	705.00	Joback Method
cpg	153.54	J/mol×K	494.86	Joback Method
cpg	164.26	J/mol×K	536.89	Joback Method
cpg	174.56	J/mol×K	578.92	Joback Method
cpg	184.39	J/mol×K	620.95	Joback Method
cpg	193.70	J/mol×K	662.97	Joback Method
cpg	210.53	J/mol×K	747.03	Joback Method
cps	129.70	J/mol×K	291.20	NIST Webbook
cps	126.40	J/mol×K	298.15	NIST Webbook
cps	132.20	J/mol×K	298.00	NIST Webbook
hfust	18.45	kJ/mol	386.00	NIST Webbook
hfust	18.40 ± 0.10	kJ/mol	385.10	NIST Webbook
hfust	18.40 ± 0.30	kJ/mol	385.70	NIST Webbook
hfust	18.45	kJ/mol	388.00	NIST Webbook
hfust	18.45	kJ/mol	388.00	NIST Webbook
hsubt	62.80	kJ/mol	269.00	NIST Webbook
hsubt	68.00 ± 0.50	kJ/mol	262.00	NIST Webbook
hvapt	47.80	kJ/mol	395.00	NIST Webbook
sfust	47.80	J/mol×K	386.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.71753e+01

Coeff. B	-4.18082e+03
Coeff. C	-1.02894e+02
Temperature range (K), min.	350.46
Temperature range (K), max.	455.30

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermochemistry of benzoquinones:	https://www.doi.org/10.1016/j.jct.2004.03.002
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106514&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume