p-Benzoquinone, 2-methyl-

Other names:	2,5-Cyclohexadiene-1,4-dione, 2-methyl-
	p-Toluquinone
	Methyl-p-benzoquinone
	Methyl-1,4-benzoquinone
	Toluquinone
	Tolylquinone
	2-Methyl-p-benzoquinone
	2-Methyl-1,4-benzoquinone
	2-Methylbenzoquinone
	2-Methylquinone
	1,4-Toluquinone
	2-Methyl-1,4-quinone
	2-Methylbenzoquinone-1,4
	2-Methyl-1,4-benzochinon
	1,4-Toluchinon
	2-Methyl-2,5-cyclohexadiene-1,4-dione
	NSC 405002
Inchi:	InChI=1S/C7H6O2/c1-5-4-6(8)2-3-7(5)9/h2-4H,1H3
InchiKey:	VTWDKFNVVLAELH-UHFFFAOYSA-N
Formula:	C7H6O2
SMILES:	CC1=CC(=O)C=CC1=O
Mol. weight [g/mol]:	122.12
CAS:	553-97-9

Physical Properties

Property code	Value	Unit	Source
chs	-3361.00	kJ/mol	NIST Webbook
ea	1.85 ± 0.06	eV	NIST Webbook
ea	1.85 ± 0.05	eV	NIST Webbook
gf	-154.67	kJ/mol	Joback Method
hf	-284.46	kJ/mol	Joback Method
hfus	5.73	kJ/mol	Joback Method
hvap	41.65	kJ/mol	Joback Method
ie	9.78 ± 0.02	eV	NIST Webbook
ie	9.78	eV	NIST Webbook
log10ws	-0.92		Crippen Method
logp	0.641		Crippen Method

mcvol	93.170	ml/mol	McGowan Method
pc	4299.92	kPa	Joback Method
rinpol	1008.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1025.00		NIST Webbook
ripol	1624.00		NIST Webbook
ripol	1616.00		NIST Webbook
ripol	1640.00		NIST Webbook
ripol	1633.00		NIST Webbook
tb	522.72	K	Joback Method
tc	771.09	K	Joback Method
tf	341.15 ± 2.00	K	NIST Webbook
vc	0.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.24	J/mol×K	522.72	Joback Method
cpg	206.10	J/mol×K	564.11	Joback Method
cpg	217.49	J/mol×K	605.51	Joback Method
cpg	228.34	J/mol×K	646.90	Joback Method
cpg	238.62	J/mol×K	688.30	Joback Method
cpg	248.26	J/mol×K	729.69	Joback Method
cpg	257.20	J/mol×K	771.09	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=C553979&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chs:	Standard solid enthalpy of combustion
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume