2,5-Cyclohexadiene-1,4-dione, 2,6-bis(1,1-dimethylethyl)-

Other names:	p-Benzoquinone, 2,6-di-tert-butyl-
	2,6-Di-tert-butylbenzoquinone
	2,6-Di-tert-butylquinone
	2,6-di-tert-Butyl-para-benzoquinone
	2,6-di-t-Butyl-p-benzoquinone
	2,6-di-tert-Butyl-p-benzoquinone
	2,6-Bis(1,1-Dimethylethyl)-2,5-cyclohexadiene-1,4-dione
	DBQ
	2,6-Di-tert-butyl-1,4-benzoquinone
	2,6-bis-tert-Butylbenzoquinone
	Benzoquinone, 2,6-di-(1,1-dimethylethyl)
	p-Benzoquinone, 2,6-bis-(1,1-dimethylethyl)
	NSC 14448
	2,6-bis-(1,1-Dimethylethyl)-2,5-cycloxehadien-1,4-dione
Inchi:	InChI=1S/C14H20O2/c1-13(2,3)10-7-9(15)8-11(12(10)16)14(4,5)6/h7-8H,1-6H3
InchiKey:	RDQSIADLBQFVMY-UHFFFAOYSA-N
Formula:	C14H20O2
SMILES:	CC(C)(C)C1=CC(=O)C=C(C(C)(C)C)C1=O
Mol. weight [g/mol]:	220.31
CAS:	719-22-2

Physical Properties

Property code	Value	Unit	Source
ea	1.87 ± 0.10	eV	NIST Webbook
gf	-99.68	kJ/mol	Joback Method
hf	-457.91	kJ/mol	Joback Method
hfus	8.64	kJ/mol	Joback Method
hvap	55.31	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.083		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1472.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1472.00		NIST Webbook

rinpol	1443.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1474.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1472.10		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1482.00		NIST Webbook
ripol	1814.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1820.00		NIST Webbook
tb	681.40	K	Joback Method
tc	924.70	K	Joback Method
tf	427.00	K	Joback Method
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.79	J/mol×K	681.40	Joback Method
cpg	557.81	J/mol×K	721.95	Joback Method
cpg	575.45	J/mol×K	762.50	Joback Method
cpg	591.74	J/mol×K	803.05	Joback Method
cpg	606.71	J/mol×K	843.60	Joback Method
cpg	620.37	J/mol×K	884.15	Joback Method
cpg	632.77	J/mol×K	924.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C719222&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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