Duroquinone

Other names:	1,4-benzoquinone, tetramethyl- 2,3,5,6-Tetramethyl-1,4-benzoquinone 2,3,5,6-Tetramethyl-2,5-cyclohexadiene-1,4-dione 2,3,5,6-Tetramethyl-p-benzoquinone 2,3,5,6-tetramethylbenzoquinone 2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetramethyl- NSC 2068 Tetramethyl-1,4-benzoquinone Tetramethyl-p-quinone Tetramethylquinone p-Benzoquinone, 2,3,5,6-tetramethyl- p-Benzoquinone, tetramethyl- p-Benzoquinone, tetramethyl-, semiquinone tetramethyl-p-benzoquinone
Inchi:	InChI=1S/C10H12O2/c1-5-6(2)10(12)8(4)7(3)9(5)11/h1-4H3
InchiKey:	WAMKWBHYPYBEJY-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC1=C(C)C(=O)C(C)=C(C)C1=O
Mol. weight [g/mol]:	164.20
CAS:	527-17-3

Physical Properties

Property code	Value	Unit	Source
ea	1.62 ± 0.06	eV	NIST Webbook
ea	1.60 ± 0.05	eV	NIST Webbook
gf	-158.30	kJ/mol	Joback Method
hf	-380.79	kJ/mol	Joback Method
hfus	18.54	kJ/mol	Thermochemistry of benzoquinones
hsub	93.20 ± 1.20	kJ/mol	NIST Webbook
hvap	50.32	kJ/mol	Joback Method
ie	9.16 ± 0.03	eV	NIST Webbook
ie	9.16 ± 0.03	eV	NIST Webbook
ie	9.25 ± 0.05	eV	NIST Webbook
ie	9.10	eV	NIST Webbook
log10ws	-2.17		Crippen Method
logp	1.811		Crippen Method

mcvol	135.440	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	606.30	K	Joback Method
tc	842.79	K	Joback Method
tf	380.00 ± 2.00	K	NIST Webbook
vc	0.515	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.72	J/mol×K	606.30	Joback Method
cpg	342.33	J/mol×K	645.71	Joback Method
cpg	356.29	J/mol×K	685.13	Joback Method
cpg	369.54	J/mol×K	724.54	Joback Method
cpg	382.03	J/mol×K	763.96	Joback Method
cpg	393.68	J/mol×K	803.37	Joback Method
cpg	404.43	J/mol×K	842.79	Joback Method
hfust	18.40 ± 0.10	kJ/mol	384.10	NIST Webbook
hfust	18.50 ± 0.10	kJ/mol	384.80	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of benzoquinones: https://www.doi.org/10.1016/j.jct.2004.03.002
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=C527173&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume