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

Other names:	p-Benzoquinone, 2,5-dimethyl-
	p-Xyloquinone
	Phlorone
	2,5-Dimethyl-p-benzoquinone
	2,5-Dimethyl-1,4-benzoquinone
	2,5-Dimethylquinone
	2,5-Xyloquinone
	3,6-Dimethyl-p-benzoquinone
	Benzoquinone, 2, 5-dimethyl-
	2,5-Dimethyl-1,4-benzochinon
	2,5-Dimetilbenzochinone (1:4)
	Floron
	Florone
	2,5-Dimethyl-2,5-Cyclohexadiene-1,4-dione
	2,5-Dimethyl-p-quinone
	NSC 15309
Inchi:	InChI=1S/C8H8O2/c1-5-3-8(10)6(2)4-7(5)9/h3-4H,1-2H3
InchiKey:	MYKLQMNSFPAPLZ-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	CC1=CC(=O)C(C)=CC1=O
Mol. weight [g/mol]:	136.15
CAS:	137-18-8

Physical Properties

Property code	Value	Unit	Source
ea	1.76 ± 0.06	eV	NIST Webbook
gf	-155.88	kJ/mol	Joback Method
hf	-316.57	kJ/mol	Joback Method
hfus	7.93	kJ/mol	Joback Method
hsub	76.99	kJ/mol	NIST Webbook
hvap	44.54	kJ/mol	Joback Method
ie	9.60 ± 0.05	eV	NIST Webbook
ie	9.58	eV	NIST Webbook
log10ws	-1.33		Crippen Method
logp	1.031		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method

rinpol	1129.00		NIST Webbook
rinpol	1129.00		NIST Webbook
tb	550.58	K	Joback Method
tc	795.00	K	Joback Method
tf	354.54	K	Joback Method
vc	0.404	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.44	J/mol×K	754.27	Joback Method
cpg	236.88	J/mol×K	550.58	Joback Method
cpg	249.76	J/mol×K	591.32	Joback Method
cpg	262.12	J/mol×K	632.05	Joback Method
cpg	273.89	J/mol×K	672.79	Joback Method
cpg	285.02	J/mol×K	713.53	Joback Method
cpg	305.11	J/mol×K	795.00	Joback Method
hsubt	77.00	kJ/mol	283.00	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C137188&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
hsub: Enthalpy of sublimation at standard conditions

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