2,5-Cyclohexadiene-1,4-dione, 2,6-dimethyl-

Other names:	p-Benzoquinone, 2,6-dimethyl-
	m-Xyloquinone
	2,6-Dimethyl-p-benzoquinone
	2,6-Dimethyl-1,4-benzoquinone
	2,6-Dimethyl-1,4-quinone
	2,6-Dimethylbenzoquinone
	2,6-Dimethylquinone
	2,6-Xyloquinone
	2,6-Dimethylbenzo-1,4-quinone
	2,6-Dimethyl-2,5-cyclohexadien-1,4-dione
	3,5-Dimethylbenzoquinone
	NSC 17549
	2,6-Dimethyl-2,5-cycloxehadien-1,4-dione
Inchi:	InChI=1S/C8H8O2/c1-5-3-7(9)4-6(2)8(5)10/h3-4H,1-2H3
InchiKey:	SENUUPBBLQWHMF-UHFFFAOYSA-N
Formula:	C8H8O2
SMILES:	CC1=CC(=O)C=C(C)C1=O
Mol. weight [g/mol]:	136.15
CAS:	527-61-7

Physical Properties

Property code	Value	Unit	Source
ea	1.76 ± 0.05	eV	NIST Webbook
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
hvap	44.54	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.031		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
rinpol	1113.00		NIST Webbook
rinpol	1119.00		NIST Webbook
rinpol	1130.00		NIST Webbook
rinpol	1125.00		NIST Webbook
ripol	1711.00		NIST Webbook

ripol	1711.00		NIST Webbook
ripol	1681.00		NIST Webbook
ripol	1686.00		NIST Webbook
ripol	1695.00		NIST Webbook
ripol	1703.00		NIST Webbook
ripol	1711.00		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	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	295.44	J/mol×K	754.27	Joback Method
cpg	305.11	J/mol×K	795.00	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C527617&Units=SI

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

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