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

Other names:	p-Benzoquinone, 2,5-dichloro-
	2,5-Dichloro-p-benzoquinone
	2,5-Dichloro-1,4-benzoquinone
	2,5-Dichloro-2,5-cyclohexa-diene-1,4-dione
	2,5-Dichoro-p-benzoquinone
	2,5-Dichlorobenzoquinone
Inchi:	InChI=1S/C6H2Cl2O2/c7-3-1-5(9)4(8)2-6(3)10/h1-2H
InchiKey:	LNXVNZRYYHFMEY-UHFFFAOYSA-N
Formula:	C6H2Cl2O2
SMILES:	O=C1C=C(Cl)C(=O)C=C1Cl
Mol. weight [g/mol]:	176.99
CAS:	615-93-0

Physical Properties

Property code	Value	Unit	Source
chs	-2448.90 ± 8.40	kJ/mol	NIST Webbook
chs	-2443.00	kJ/mol	NIST Webbook
ea	2.37 ± 0.05	eV	NIST Webbook
ea	2.44 ± 0.06	eV	NIST Webbook
gf	-196.58	kJ/mol	Joback Method
hf	-306.77	kJ/mol	Joback Method
hfs	-255.00	kJ/mol	NIST Webbook
hfus	11.14	kJ/mol	Joback Method
hvap	48.86	kJ/mol	Joback Method
ie	10.24 ± 0.03	eV	NIST Webbook
log10ws	-1.79		Crippen Method
logp	1.384		Crippen Method
mcvol	103.560	ml/mol	McGowan Method
pc	4339.67	kPa	Joback Method
tb	579.68	K	Joback Method
tc	843.27	K	Joback Method
tf	391.84	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.18	J/mol×K	579.68	Joback Method
cpg	202.21	J/mol×K	623.61	Joback Method
cpg	210.81	J/mol×K	667.54	Joback Method
cpg	218.88	J/mol×K	711.47	Joback Method
cpg	226.34	J/mol×K	755.40	Joback Method
cpg	233.14	J/mol×K	799.34	Joback Method
cpg	239.18	J/mol×K	843.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C615930&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

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
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume