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

Other names:	2,6-Dichloquinone
	2,6-Dichloro-1,4-benzoquinone
	2,6-Dichloro-2,5-cyclohexa-diene-1,4-dione
	2,6-Dichloro-p-benzoquinone
	2,6-Dichlorobenzoquinone
	2,6-Dichloroquinone
	NSC 6211
	p-Benzoquinone, 2,6-dichloro-
	p-Quinone, 2,6-dichloro-
Inchi:	InChI=1S/C6H2Cl2O2/c7-4-1-3(9)2-5(8)6(4)10/h1-2H
InchiKey:	JCARTGJGWCGSSU-UHFFFAOYSA-N
Formula:	C6H2Cl2O2
SMILES:	O=C1C=C(Cl)C(=O)C(Cl)=C1
Mol. weight [g/mol]:	176.99
CAS:	697-91-6

Physical Properties

Property code	Value	Unit	Source
chs	-2449.70 ± 8.40	kJ/mol	NIST Webbook
chs	-2422.00	kJ/mol	NIST Webbook
chs	-2444.00	kJ/mol	NIST Webbook
ea	2.48 ± 0.05	eV	NIST Webbook
ea	2.48 ± 0.06	eV	NIST Webbook
gf	-196.58	kJ/mol	Joback Method
hf	-306.77	kJ/mol	Joback Method
hfs	-254.00	kJ/mol	NIST Webbook
hfus	11.14	kJ/mol	Joback Method
hsub	69.90 ± 8.40	kJ/mol	NIST Webbook
hvap	48.86	kJ/mol	Joback Method
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	233.14	J/mol×K	799.34	Joback Method
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	239.18	J/mol×K	843.27	Joback Method
hsubt	69.90 ± 8.30	kJ/mol	294.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.09045e+01
Coeff. B	-8.54951e+03
Temperature range (K), min.	414.68
Temperature range (K), max.	548.29

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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=C697916&Units=SI

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

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