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

Other names:	2-Chloro-1,4-benzoquinone
	2-Chloro-2,5-cyclohexadien-1,4-dione
	2-Chloro-p-benzoquinone
	2-Chloroquinone
	Chloro-1,4-benzoquinone
	Chloro-p-benzoquinone
	Chloroquinone
	Monochloro-p-benzoquinone
	Monochlorobenzoquinone
	Monochloroquinone
	NSC 526777
	p-Benzoquinone, 2-chloro-
	p-Benzoquinone, chloro-
Inchi:	InChI=1S/C6H3ClO2/c7-5-3-4(8)1-2-6(5)9/h1-3H
InchiKey:	WOGWYSWDBYCVDY-UHFFFAOYSA-N
Formula:	C6H3ClO2
SMILES:	O=C1C=CC(=O)C(Cl)=C1
Mol. weight [g/mol]:	142.54
CAS:	695-99-8

Physical Properties

Property code	Value	Unit	Source
chs	-2580.00	kJ/mol	NIST Webbook
chs	-2590.00	kJ/mol	NIST Webbook
chs	-2592.80 ± 8.40	kJ/mol	NIST Webbook
gf	-175.02	kJ/mol	Joback Method
hf	-279.56	kJ/mol	Joback Method
hfs	-231.00	kJ/mol	NIST Webbook
hfus	7.33	kJ/mol	Joback Method
hsub	69.04	kJ/mol	NIST Webbook
hvap	43.81	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	0.817		Crippen Method
mcvol	91.320	ml/mol	McGowan Method
pc	4652.99	kPa	Joback Method
tb	537.27	K	Joback Method
tc	795.71	K	Joback Method

tf	349.40	K	Joback Method
vc	0.341	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.73	J/mol×K	752.64	Joback Method
cpg	174.23	J/mol×K	537.27	Joback Method
cpg	184.11	J/mol×K	580.34	Joback Method
cpg	193.57	J/mol×K	623.42	Joback Method
cpg	202.53	J/mol×K	666.49	Joback Method
cpg	210.94	J/mol×K	709.57	Joback Method
cpg	225.83	J/mol×K	795.71	Joback Method
hsubt	69.00 ± 8.30	kJ/mol	276.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.17617e+01
Coeff. B	-7.98104e+03
Temperature range (K), min.	371.66
Temperature range (K), max.	485.16

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C695998&Units=SI

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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
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