p-Benzoquinone, 2,3,5,6-tetrachloro-

Other names:
.alpha.-chloranil
1,2,4,5-tetrachlorobenzoquinone
1,4-Benzoquinone, 2,3,5,6-tetrachloro-
1,4-benzoquinone, tetrachloro-
2,3,5,6-Tetrachloro-1,4-benzoquinone
2,3,5,6-Tetrachloro-2,5-cyclohexadiene-1,4-dione
2,3,5,6-Tetrachloro-p-benzoquinone
2,3,5,6-Tetrachlorobenzoquinone
2,3,5,6-Tetrachloroquinone
2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrachloro-
Chloranil
Coversan
Dow Seed Disinfectant No. 5
ENT 3,797
ENT 3797
G-25804
G-444E
Geigy-444e
Khloranil
NSC 8432
Psorisan
Quinone Tetrachloride
Reranil
Spergon
Spergon I
Spergon Technical
Tetrachloro-1,4-benzoquinone
Tetrachloro-p-benzoquinone
Tetrachloro-p-quinone
Tetrachlorobenzoquinone
Tetrachloroparabenzoquinone
Tetrachloroquinone
Tetrachlorquinone
Vulklor
p-Chloranil
«alpha»-Chloranil
Â«alphaÂ»-Chloranil

Inchi: InChI=1S/C6Cl4O2/c7-1-2(8)6(12)4(10)3(9)5(1)11

InchiKey: UGNWTBMOAKPKBL-UHFFFAOYSA-N

Formula: C6Cl4O2

SMILES: O=C1C(Cl)=C(Cl)C(=O)C(Cl)=C1Cl
Mol. weight [g/mol]: 245.88
CAS: 118-75-2

Physical Properties

Property code	Value	Unit	Source
chs	-2171.10 ± 8.40	kJ/mol	NIST Webbook
chs	-2156.00	kJ/mol	NIST Webbook
chs	-2166.00	kJ/mol	NIST Webbook
ea	2.45 ± 0.26	eV	NIST Webbook
ea	2.76 ± 0.20	eV	NIST Webbook
ea	2.75 ± 0.05	eV	NIST Webbook
ea	2.78 ± 0.10	eV	NIST Webbook
gf	-239.70	kJ/mol	Joback Method
hf	-361.19	kJ/mol	Joback Method
hfs	-298.00	kJ/mol	NIST Webbook
hfus	18.76	kJ/mol	Joback Method
hsub	98.74	kJ/mol	NIST Webbook
hvap	58.95	kJ/mol	Joback Method
ie	9.90 ± 0.05	eV	NIST Webbook
ie	9.74	eV	NIST Webbook
log10ws	-3.09		Crippen Method
logp	2.517		Crippen Method
mcvol	128.040	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
ss	258.40	J/mol×K	NIST Webbook
tb	664.50	K	Joback Method
tc	935.65	K	Joback Method
tf	568.13 ± 0.20	K	NIST Webbook
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.77	J/mol×K	890.46	Joback Method
cpg	226.43	J/mol×K	664.50	Joback Method
cpg	233.75	J/mol×K	709.69	Joback Method

cpg	240.55	J/mol×K	754.88	Joback Method
cpg	246.72	J/mol×K	800.07	Joback Method
cpg	252.16	J/mol×K	845.26	Joback Method
cpg	260.45	J/mol×K	935.65	Joback Method
cps	193.80	J/mol×K	298.15	NIST Webbook
hfust	30.87	kJ/mol	567.20	NIST Webbook
hfust	30.87	kJ/mol	567.20	NIST Webbook
hsubt	98.70 ± 8.30	kJ/mol	344.50	NIST Webbook
hvapt	88.50	kJ/mol	389.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.57544e+01
Coeff. B	-1.19044e+04
Temperature range (K), min.	467.45
Temperature range (K), max.	582.32

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Spectroscopic and ultrasonic studies on the molecular interaction of certain aromatic amines with p-chloranil: https://www.doi.org/10.1016/j.fluid.2013.09.026

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=C118752&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

Legend

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

cps: Solid phase 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
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume