Tetrachloro-o-benzoquinone

Other names:	3,5-Cyclohexadiene-1,2-dione, 3,4,5,6-tetrachloro- o-Benzoquinone, 3,4,5,6-tetrachloro- o-Chloranil o-Chloroanil Isochloranil Tetrachloro-o-quinone Tetrachloro-1,2-benzoquinone 3,4,5,6-Tetrachloro-o-benzoquinone 3,4,5,6-Tetrachloro-1,2-benzoquinone 3,4,5,6-Tetrachloro-3,5-cyclohexadiene-1,2-dione ortho-Chloranil NSC 403503 2-Chloranil
Inchi:	InChI=1S/C6Cl4O2/c7-1-2(8)4(10)6(12)5(11)3(1)9
InchiKey:	VRGCYEIGVVTZCC-UHFFFAOYSA-N
Formula:	C6Cl4O2
SMILES:	O=C1C(=O)C(Cl)=C(Cl)C(Cl)=C1Cl
Mol. weight [g/mol]:	245.88
CAS:	2435-53-2

Physical Properties

Property code	Value	Unit	Source
gf	-239.70	kJ/mol	Joback Method
hf	-361.19	kJ/mol	Joback Method
hfus	18.76	kJ/mol	Joback Method
hvap	58.95	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.517		Crippen Method
mcvol	128.040	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	664.50	K	Joback Method
tc	935.65	K	Joback Method
tf	476.72	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	256.77	J/mol×K	890.46	Joback Method
cpg	260.45	J/mol×K	935.65	Joback Method

Sources

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=C2435532&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume