

3,5-Cyclohexadiene-1,2-dione, 3,4,5,6-tetrachloro-

Other names:	2-Chloranil 3,4,5,6-Tetrachloro-1,2-benzoquinone 3,4,5,6-Tetrachloro-3,5-cyclohexadiene-1,2-dione 3,4,5,6-Tetrachloro-o-benzoquinone 3,5-Cyclohexadiene-1,2-dione, 3,4,5,6-tetrachloro- Isochloranil NSC 403503 Tetrachloro-1,2-benzoquinone Tetrachloro-o-quinone o-Benzoquinone, 3,4,5,6-tetrachloro- o-Chloranil o-Chloroanil ortho-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

Physical Properties

Property code	Value	Unit	Source
hfus	18.76	kJ/mol	Joback Method
ie	9.59	eV	Cheméo Relay (1.0)
logp	2.517		Crippen Method
mcvol	128.040	ml/mol	McGowan Method
tf	522.97	K	Cheméo Relay (1.0)

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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2435532&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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