1,2-Dichloro-4,5-dicyano-p-benzoquinone

Other names:	1,4-Cyclohexadiene-1,2-dicarbonitrile, 4,5-dichloro-3,6-dioxo-
	Dichlorodicyano-p-benzoquinone
	Dichlorodicyanobenzoquinone
	Dichlorodicyanoquinone
	DDQ
	1,2-Dichloro-4,5-dicyanobenzoquinone
	2,3-Dichloro-5,6-dicyanobenzoquinone
	2,3-Dichloro-5,6-dicyanoquinone
	2,3-Dicyano-5,6-dichlorobenzoquinone
	2,3,5,6-Dichlorodicyanoquinone
	2,3-Dichloro-5,6-dicyano-1,4-benzoquinone
	2,3-Dichloro-5,6-dicyano-para-benzoquinone
	2,3-Dichloro-5,6-dicyano-p-benzoquinone
	4,5-Dichloro-3,6-dioxo-1,4-cyclohexadiene-1,2-dicarbonitrile
	2,3-Dichloro-5,6-dicyano-p-quinone
	2,3-Dicyano-5,6-dichloro-1,4-benzoquinone
	5,6-Dichloro-2,3-dicyano-p-benzoquinone
	5,6-Dicyano-2,3-dichloro-p-benzoquinone
	NSC 401087
	4,5-dichloro-3,6-dioxocyclohexa-1,4-diene-1,2-dicarbonitrile
Inchi:	InChI=1S/C8Cl2N2O2/c9-5-6(10)8(14)4(2-12)3(1-11)7(5)13
InchiKey:	HZNVUJQVZSTENZ-UHFFFAOYSA-N
Formula:	C8Cl2N2O2
SMILES:	N#CC1=C(C#N)C(=O)C(Cl)=C(Cl)C1=O
Mol. weight [g/mol]:	227.00
CAS:	84-58-2

Physical Properties

Property code	Value	Unit	Source
gf	67.36	kJ/mol	Joback Method
hf	-41.23	kJ/mol	Joback Method
hfus	18.55	kJ/mol	Joback Method
hvap	75.59	kJ/mol	Joback Method
ie	10.58 ± 0.05	eV	NIST Webbook
log10ws	-2.36		Crippen Method
logp	1.171		Crippen Method
mcvol	134.500	ml/mol	McGowan Method

pc	3121.00	kPa	Joback Method
tb	839.56	K	Joback Method
tc	1111.77	K	Joback Method
tf	569.40	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	288.28	J/mol×K	839.56	Joback Method
cpg	293.95	J/mol×K	884.93	Joback Method
cpg	298.59	J/mol×K	930.30	Joback Method
cpg	302.09	J/mol×K	975.67	Joback Method
cpg	304.36	J/mol×K	1021.04	Joback Method
cpg	305.28	J/mol×K	1066.41	Joback Method
cpg	304.75	J/mol×K	1111.77	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C84582&Units=SI
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

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
ie: Ionization energy
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