Dichlone

Other names:	1,4-naphthalenedione, 2,3-dichloro-
	1,4-naphthoquinone, 2,3-dichloro-
	2,3-Dichlor-1,4-naftochinon
	2,3-Dichlor-1,4-naphthochinon
	2,3-Dichloro-1,4-naphthaquinone
	2,3-Dichloro-1,4-naphthoquinone (dichlone)
	2,3-Dichloro-«alpha»-naphthoquinone
	2,3-Dichloronaphthoquinone
	2,3-Dichloronaphthoquinone-1,4
	2,3-dichloro-1,4-naphthalenedione
	2,3-dichloro-1,4-naphthoquinone
	Algistat
	CNQ
	Compound 604
	Dichloronaphthoquinone
	Diclone
	ENT 3,776
	Latka 604
	NSC 537
	Phygon
	Phygon Seed Protectant
	Phygon XL
	Phygon paste
	Quintar
	Quintar 540F
	Sanquinon
	U.S. rubber 604
	USR 604
	Uniroyal
Inchi:	InChI=1S/C10H4Cl2O2/c11-7-8(12)10(14)6-4-2-1-3-5(6)9(7)13/h1-4H
InchiKey:	SVPKNMBRVBMTLB-UHFFFAOYSA-N
Formula:	C10H4Cl2O2
SMILES:	O=C1C(Cl)=C(Cl)C(=O)c2ccccc21
Mol. weight [g/mol]:	227.04
CAS:	117-80-6

Physical Properties

Property code	Value	Unit	Source
ea	2.21 ± 0.10	eV	NIST Webbook
gf	-65.88	kJ/mol	Joback Method
hf	-209.73	kJ/mol	Joback Method
hfus	18.13	kJ/mol	Joback Method
hvap	60.07	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
ie	9.67 ± 0.02	eV	NIST Webbook
log10ws	-3.84		Crippen Method
logp	2.755		Crippen Method
mcvol	140.460	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	695.16	K	Joback Method
tc	968.50	K	Joback Method
tf	469.56 ± 0.20	K	NIST Webbook
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.43	J/mol×K	695.16	Joback Method
cpg	322.36	J/mol×K	740.72	Joback Method
cpg	332.36	J/mol×K	786.27	Joback Method
cpg	341.39	J/mol×K	831.83	Joback Method
cpg	349.43	J/mol×K	877.39	Joback Method
cpg	356.46	J/mol×K	922.94	Joback Method
cpg	362.44	J/mol×K	968.50	Joback Method
hfust	28.53	kJ/mol	469.00	NIST Webbook
hfust	28.53	kJ/mol	469.00	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Solubility of menadione and dichlone in supercritical carbon dioxide: https://www.doi.org/10.1016/j.fluid.2016.04.001

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=C117806&Units=SI

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume