9,10-Anthracenedione, 1-chloro-

Other names:	1-Chloranthrachinon
	1-Chloro-9,10-anthraquinone
	1-Chloroanthraquinone
	Anthraquinone, 1-chloro-
	chloroanthraquinone
	«alpha»-Chloroanthraquinone
	«alpha»-Monochloroanthraquinone
	Â«alphaÂ»-Chloroanthraquinone
	Â«alphaÂ»-Monochloroanthraquinone
Inchi:	InChI=1S/C14H7ClO2/c15-11-7-3-6-10-12(11)14(17)9-5-2-1-4-8(9)13(10)16/h1-7H
InchiKey:	BOCJQSFSGAZAPQ-UHFFFAOYSA-N
Formula:	C14H7ClO2
SMILES:	O=C1c2ccccc2C(=O)c2c(Cl)cccc21
Mol. weight [g/mol]:	242.66
CAS:	82-44-0

Physical Properties

Property code	Value	Unit	Source
ea	1.71 ± 0.06	eV	NIST Webbook
gf	86.38	kJ/mol	Joback Method
hf	-85.48	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	66.22	kJ/mol	Joback Method
log10ws	-5.54		Aqueous Solubility Prediction Method
logp	3.115		Crippen Method
mcvol	165.120	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
tb	768.23	K	Joback Method
tc	1045.44	K	Joback Method
tf	434.65	K	Aqueous Solubility Prediction Method
tf	435.20	K	Solubility Measurement and Modeling for 2-Benzoyl-3-chlorobenzoic Acid and 1-Chloroanthraquinone in Organic Solvents
vc	0.632	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.60	J/mol×K	768.23	Joback Method
cpg	434.19	J/mol×K	814.43	Joback Method
cpg	445.60	J/mol×K	860.63	Joback Method
cpg	455.86	J/mol×K	906.84	Joback Method
cpg	465.03	J/mol×K	953.04	Joback Method
cpg	473.13	J/mol×K	999.24	Joback Method
cpg	480.23	J/mol×K	1045.44	Joback Method

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C82440&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility Measurement and Modeling for 2-Benzoyl-3-chlorobenzoic Acid and 1-Chloroanthraquinone in Organic Solvents:	https://www.doi.org/10.1021/je400246s
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
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