Chloroxine

Other names:	5,7-Dichlor-8-hydroxychinolin 5,7-Dichloro-8-Hydroxyquinoline 5,7-Dichloro-8-hydroquinoline 5,7-Dichloro-8-oxyquinoline 5,7-Dichloro-8-quinolinol 5,7-Dichlorooxine 5,7-Dichloroxine 5,7-dichloroquinolin-8-ol 8-Quinolinol, 5,7-dichloro- CHQ Capitrol Chlofucid Chloroxyquinoline Chlorquinol Clofuzid Dichlorohydroxyquinoline Dichloroquinolinol Dichloroxin Dikhloroskin Endiaron NSC 3904 Quesyl Quinolor Quixalin
Inchi:	InChI=1S/C9H5Cl2NO/c10-6-4-7(11)9(13)8-5(6)2-1-3-12-8/h1-4,13H
InchiKey:	WDFKMLRRRCGAKS-UHFFFAOYSA-N
Formula:	C9H5Cl2NO
SMILES:	Oc1c(Cl)cc(Cl)c2cccnc12
Mol. weight [g/mol]:	214.05
CAS:	773-76-2

Physical Properties

Property code	Value	Unit	Source
chs	-4145.30 ± 1.30	kJ/mol	NIST Webbook
hf	-48.80 ± 1.90	kJ/mol	NIST Webbook
hfs	-158.10 ± 1.80	kJ/mol	NIST Webbook

hsub	92.90 ± 0.80	kJ/mol	NIST Webbook
hsub	109.30 ± 0.70	kJ/mol	NIST Webbook
log10ws	-3.96		Crippen Method
logp	3.247		Crippen Method
mcvol	134.780	ml/mol	McGowan Method
tt	452.15	K	Solid-Liquid Equilibrium of 5-Chloro-8-hydroxyquinoline and 5,7-Dichloro-8-hydroxyquinoline in Different Solvents and Mixing Properties of Solutions

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	106.30 ± 0.70	kJ/mol	358.50	NIST Webbook
hsubt	92.90	kJ/mol	378.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.39584e+01
Coeff. B	-1.11906e+04
Temperature range (K), min.	472.76
Temperature range (K), max.	600.13

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solubility of chloroxine in aqueous co-solvent mixtures of N,N-dimethylformamide, dimethyl sulfoxide, N-methyl-2-pyrrolidone and 1,4-dioxane, Determination, solvent effect and preferential solvation analysis:	https://www.doi.org/10.1016/j.jct.2019.07.001
Cosolvency and Mathematical Modeling Analysis of Chloroxine in Solid-Liquid Equilibrium of 5-Chloro-8-hydroxyquinoline and 5,7-Dichloro-8-hydroxyquinoline in Different Solvents and Mixing Properties of Solutions:	https://www.doi.org/10.1021/acs.jced.8b00257
Solid-Liquid Equilibrium of 5-Chloro-8-hydroxyquinoline and 5,7-Dichloro-8-hydroxyquinoline in Different Solvents and Mixing Properties of Solutions:	https://www.doi.org/10.1021/acs.jced.9b00028
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C773762&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tt:	Triple Point Temperature

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