

Cloxyquin

Other names: 5-Chloro-8-oxyquinoline
5-Chloro-8-quinolol
5-Chloro-quinoline-8-ol
5-Chlorooxine
5-Chloroquinolin-8-ol
5-chloro-8-hydroxyquinoline
5-chloro-8-quinolinol
8-Hydroxy-5-chloroquinoline
8-Quinolinol, 5-chloro-
Chlorisept
Cloxiquine
Dermofongin
Dermofungin
NSC 35083
quinoline, 5-chloro-8-hydroxy-

Inchi: InChI=1S/C9H6ClNO/c10-7-3-4-8(12)9-6(7)2-1-5-11-9/h1-5,12H

InchiKey: CTQMJYWVDVABFRZ-UHFFFAOYSA-N

Formula: C9H6ClNO

SMILES: Oc1ccc(Cl)c2cccnc12

Mol. weight [g/mol]: 179.60

CAS: 130-16-5

Physical Properties

Property code	Value	Unit	Source
chs	-4298.50 ± 1.40	kJ/mol	NIST Webbook
hf	-25.50 ± 2.10	kJ/mol	NIST Webbook
hfs	-124.20 ± 1.90	kJ/mol	NIST Webbook
hsub	98.70 ± 0.90	kJ/mol	NIST Webbook
log10ws	-3.27		Crippen Method
logp	2.594		Crippen Method
mcvol	122.540	ml/mol	McGowan Method
tf	343.15 ± 2.00	K	NIST Webbook
tt	395.48	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	97.50 ± 0.90	kJ/mol	322.00	NIST Webbook

Sources

Crippen Method:

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

Solid-Liquid Equilibrium of
5-Chloro-8-hydroxyquinoline and
N-Quinoline-8-hydroxyquinoline in
Different Solvents and Mixing
Properties of Solutions:

<https://www.doi.org/10.1021/acs.jced.9b00028>

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C130165&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature

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