Quinoline, 4,7-dichloro-

Other names:	4,7-Dichloroquinoline
	TL 1473
Inchi:	InChI=1S/C9H5Cl2N/c10-6-1-2-7-8(11)3-4-12-9(7)5-6/h1-5H
InchiKey:	HXEWMTXDBOQQKO-UHFFFAOYSA-N
Formula:	C9H5Cl2N
SMILES:	Clc1ccc2c(Cl)ccnc2c1
Mol. weight [g/mol]:	198.05
CAS:	86-98-6

Physical Properties

Property code	Value	Unit	Source
hsub	89.50 ± 2.30	kJ/mol	NIST Webbook
log10ws	-2.80		Aqueous Solubility Prediction Method
logp	3.542		Crippen Method
mcvol	128.910	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86986&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubility of Chloroquine Diphosphate and 4,7-Dichloroquinoline in Water, Ethanol, Tetrahydrofuran, Acetonitrile, and Acetone from (298.2 to 333.2) K:	https://www.doi.org/10.1021/je8007099
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume