

# quinhydrone

**Inchi:** InChI=1S/C6H6O2.C6H4O2/c2\*7-5-1-2-6(8)4-3-5/h1-4,7-8H;1-4H  
**InchiKey:** BDJXVNRFAQSMAA-UHFFFAOYSA-N  
**Formula:** C12H10O4  
**SMILES:** O=C1C=CC(=O)C=C1.Oc1ccc(O)cc1  
**Mol. weight [g/mol]:** 218.21  
**CAS:** 106-34-3

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.73		Aqueous Solubility Prediction Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	228.40	J/molxK	243.40	NIST Webbook
hsubt	89.10	kJ/mol	325.50	NIST Webbook
hsubt	89.00 ± 1.00	kJ/mol	313.00	NIST Webbook

## Sources

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C106343&Units=SI>

## Legend

**cps:** Solid phase heat capacity  
**hsubt:** Enthalpy of sublimation at a given temperature  
**log10ws:** Log10 of Water solubility in mol/l

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