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

Physical Properties

Property code	Value	Unit	Source
hf	-420.37	kJ/mol	Cheméo Relay (1.0)
hvap	134.83	kJ/mol	Cheméo Relay (1.0)
ie	8.41	eV	Cheméo Relay (1.0)
log10ws	-1.73		Aqueous Solubility Prediction Method
pc	5053.85	kPa	Cheméo Relay (1.0, beta)
tb	636.63	K	Cheméo Relay (1.0)
tc	894.97	K	Cheméo Relay (1.0)
tf	477.44	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	228.40	J/mol×K	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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cps:	Solid phase heat capacity
hf:	Enthalpy of formation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point