1,4-Naphthalenedione, 5-hydroxy-

Other names:	1,4-Dihydro-1,4-dioxo-5-hydroxynaphthalene
	1,4-Naphthoquinone, 5-hydroxy-
	1,4-Naphthoquinone, 8-hydroxy-
	5-Hydroxy-1,4-naftochinon
	5-Hydroxy-1,4-naphthalenedione
	5-Hydroxy-p-naphthoquinone
	5-Hydroxynaphthoquinone
	5-hydroxy-1,4-naphthoquinone
	5-hydroxynaphthalene-1,4-dione
	8-Hydroxy-1,4-naphthalenedione
	8-Hydroxy-1,4-naphthoquinone
	Akhnot
	C.I. 75500
	C.I. Natural Brown 7
	Iuglon
	Juglane
	Juglon
	Jugnlon
	NCI 2323
	NSC 153189
	NSC 622948
	Nucin
	Regianin
	Walnut Extract
	Yuglon
	juglone
Inchi:	InChI=1S/C10H6O3/c11-7-4-5-9(13)10-6(7)2-1-3-8(10)12/h1-5,12H
InchiKey:	KQPYUDDGWXQXHS-UHFFFAOYSA-N
Formula:	C10H6O3
SMILES:	O=C1C=CC(=O)c2c(O)cccc21
Mol. weight [g/mol]:	174.16

Physical Properties

Property code	Value	Unit	Source
hf	-320.75	kJ/mol	Cheméo Relay (1.0)
hfus	16.30	kJ/mol	Joback Method

ie	8.60	eV	NIST Webbook
ie	8.70 ± 0.02	eV	NIST Webbook
ie	8.85	eV	NIST Webbook
log10ws	-2.64		Cheméo Relay (1.0)
logp	1.327		Crippen Method
mcvol	121.850	ml/mol	McGowan Method
tb	570.04	K	Cheméo Relay (1.0)
tf	408.80	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.20	J/mol×K	690.96	Joback Method
cpg	325.85	J/mol×K	736.68	Joback Method
cpg	336.61	J/mol×K	782.40	Joback Method
cpg	346.57	J/mol×K	828.12	Joback Method
cpg	355.79	J/mol×K	873.84	Joback Method
cpg	364.32	J/mol×K	919.56	Joback Method
cpg	372.25	J/mol×K	965.28	Joback Method

Sources

Measurement and correlation of the solubility of juglone in supercritical carbon dioxide: https://www.doi.org/10.1016/j.fluid.2011.08.024

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C481390&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity

hf: Enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point