1,4-Naphthalenedione, 5-hydroxy-2-methyl-

Other names:	1,4-Naphthoquinone, 5-hydroxy-2-methyl-
	2-Methyl-5-hydroxy-1,4-naphthoquinone
	2-Methyljuglone
	5-hydroxy-2-methyl-1,4-naphthalenedione
	5-hydroxy-2-methyl-1,4-naphthoquinone
	NSC 236613
	NSC 688284
	Plumbaein
	Plumbagine
	Plumbagone
	plumbagin
Inchi:	InChI=1S/C11H8O3/c1-6-5-9(13)10-7(11(6)14)3-2-4-8(10)12/h2-5,12H,1H3
InchiKey:	VCMMXZQDRFWYSE-UHFFFAOYSA-N
Formula:	C11H8O3
SMILES:	CC1=CC(=O)c2c(O)cccc2C1=O
Mol. weight [g/mol]:	188.18

Physical Properties

Property code	Value	Unit	Source
hf	-342.27	kJ/mol	Cheméo Relay (1.0)
hfus	18.50	kJ/mol	Joback Method
ie	8.64	eV	Cheméo Relay (1.0)
log10ws	-2.98		Cheméo Relay (1.0)
logp	1.718		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
tf	405.66	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.03	J/mol×K	718.82	Joback Method
cpg	374.36	J/mol×K	763.53	Joback Method

cpg	385.83	J/mol×K	808.23	Joback Method
cpg	396.48	J/mol×K	852.94	Joback Method
cpg	406.37	J/mol×K	897.65	Joback Method
cpg	415.56	J/mol×K	942.36	Joback Method
cpg	424.10	J/mol×K	987.06	Joback Method

Sources

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):	
Measurement and Correlation of Solubilities of 1,4-Naphthoquinone and of Plumbagin in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je200675g
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C481425&Units=SI

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
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point