Plumbagin

Other names:	1,4-Naphthalenedione, 5-hydroxy-2-methyl-
	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
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
CAS:	481-42-5

Physical Properties

Property code	Value	Unit	Source
gf	-178.59	kJ/mol	Joback Method
hf	-364.73	kJ/mol	Joback Method
hfus	18.50	kJ/mol	Joback Method
hvap	65.87	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	1.718		Crippen Method
mcvol	135.940	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method
rinpol	1600.00		NIST Webbook
rinpol	1600.00		NIST Webbook
tb	718.82	K	Joback Method
tc	987.06	K	Joback Method
tf	532.77	K	Joback Method
vc	0.460	m3/kmol	Joback Method

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C481425&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and Correlation of 1,4-Naphthoquinone and of Plumbagin Solubilities in Supercritical Carbon Dioxide:	https://www.doi.org/10.1021/je200675g

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume