2,6-Dimethoxybenzoquinone

Other names:	2,6-Dimethoxy-p-benzoquinone
	2,6-Dimethoxy-1,4-benzoquinone
	2,5-Cyclohexadiene-1,4-dione, 2,6-dimethoxy-
	p-Benzoquinone, 2,6-dimethoxy-
	2,6-Dimethoxy-p-quinone
	2,6-Dimethoxyquinone
	56336
	2,6-Dimethoxybenzo-1,4-quinone
	2,6-Dimethoxy-2,5-cyclohexadiene-1,4-dione
	3,5-Dimethoxy-1,4-benzoquinone
	NSC 24500
	Quinone, 2,6-dimethoxy-
Inchi:	InChI=1S/C8H8O4/c1-11-6-3-5(9)4-7(12-2)8(6)10/h3-4H,1-2H3
InchiKey:	OLBNOBQOQZRLMP-UHFFFAOYSA-N
Formula:	C8H8O4
SMILES:	COC1=CC(=O)C=C(OC)C1=O
Mol. weight [g/mol]:	168.15
CAS:	530-55-2

Physical Properties

Property code	Value	Unit	Source
ea	1.72 ± 0.06	eV	NIST Webbook
gf	-365.88	kJ/mol	Joback Method
hf	-581.01	kJ/mol	Joback Method
hfus	10.30	kJ/mol	Joback Method
hvap	49.36	kJ/mol	Joback Method
log10ws	-0.50		Crippen Method
logp	0.199		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
pc	3585.64	kPa	Joback Method
rinpol	1506.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1522.00		NIST Webbook
tb	595.42	K	Joback Method
tc	832.63	K	Joback Method
tf	399.00	K	Joback Method

vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.34	J/mol×K	595.42	Joback Method
cpg	295.17	J/mol×K	634.95	Joback Method
cpg	307.48	J/mol×K	674.49	Joback Method
cpg	319.18	J/mol×K	714.02	Joback Method
cpg	330.18	J/mol×K	753.56	Joback Method
cpg	340.39	J/mol×K	793.09	Joback Method
cpg	349.70	J/mol×K	832.63	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=C530552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
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