2,6-Dimethoxy-P-benzoquinone

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

Physical Properties

Property code	Value	Unit	Source
ea	1.72 ± 0.06	eV	NIST Webbook
hfus	10.30	kJ/mol	Joback Method
ie	9.07	eV	Cheméo Relay (1.0)
logp	0.199		Crippen Method
mcvol	119.000	ml/mol	McGowan Method
rinpol	1506.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1522.00		NIST Webbook
rinpol	1530.00		NIST Webbook

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
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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C530552&Units=SI

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices