2,5-Cyclohexadiene-1,4-dione, 2,3-dimethoxy-5-methyl-

Other names: p-Benzoquinone, 2,3-dimethoxy-5-methyl-
Coenzyme Q0
CoQ0
Q0
Ubiquinone Q0
Ubiquinone 0
2-Methyl-5,6-dimethoxybenzoquinone
2,3-Dimethoxy-5-methyl-p-benzoquinone
2,3-Dimethoxy-5-methyl-1,4-benzoquinone
2,3-Dimethoxy-5-methylbenzoquinone
2,3-Dimethoxy-6-methyl-p-benzoquinone
2-Methyl-4,5-dimethoxy-p-quinone

Inchi: InChI=1S/C9H10O4/c1-5-4-6(10)8(12-2)9(13-3)7(5)11/h4H,1-3H3

InchiKey: UIXPTCZPFCVOQF-UHFFFAOYSA-N

Formula: C9H10O4

SMILES: COC1=C(OC)C(=O)C(C)=CC1=O

Mol. weight [g/mol]: 182.17

CAS: 605-94-7

Physical Properties

Property code	Value	Unit	Source
ea	1.86 ± 0.06	eV	NIST Webbook
gf	-367.09	kJ/mol	Joback Method
hf	-613.12	kJ/mol	Joback Method
hfus	12.50	kJ/mol	Joback Method
hvap	52.25	kJ/mol	Joback Method
log10ws	-0.92		Crippen Method
logp	0.589		Crippen Method
mcvol	133.090	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
tb	623.28	K	Joback Method
tc	856.64	K	Joback Method
tf	422.79	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.72	J/mol×K	623.28	Joback Method
cpg	342.38	J/mol×K	662.17	Joback Method
cpg	355.45	J/mol×K	701.07	Joback Method
cpg	367.81	J/mol×K	739.96	Joback Method
cpg	379.39	J/mol×K	778.86	Joback Method
cpg	390.08	J/mol×K	817.75	Joback Method
cpg	399.80	J/mol×K	856.64	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C605947&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume