3,3',5,5'-Tetramethoxy-4,4'-diphenoquinone

Other names: Cerulignone
Inchi: InChI=1S/C16H16O6/c1-19-11-5-9(6-12(20-2)15(11)17)10-7-13(21-3)16(18)14(8-10)22-4
InchiKey: WASNBVDBYSQBPH-UHFFFAOYSA-N
Formula: C16H16O6
SMILES: COC1=CC(=C2C=C(OC)C(=O)C(OC)=C2)C=C(OC)C1=O
Mol. weight [g/mol]: 304.29
CAS: 493-74-3

Physical Properties

Property code	Value	Unit	Source
chs	-7496.10	kJ/mol	NIST Webbook
gf	-425.00	kJ/mol	Joback Method
hf	-808.45	kJ/mol	Joback Method
hfs	-1084.00	kJ/mol	NIST Webbook
hfus	26.27	kJ/mol	Joback Method
hvap	76.25	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.570		Crippen Method
mcvol	219.700	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
tb	864.92	K	Joback Method
tc	1104.43	K	Joback Method
tf	597.60	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.18	J/mol×K	864.92	Joback Method
cpg	674.69	J/mol×K	904.84	Joback Method
cpg	686.33	J/mol×K	944.76	Joback Method
cpg	695.98	J/mol×K	984.68	Joback Method
cpg	703.52	J/mol×K	1024.60	Joback Method
cpg	708.81	J/mol×K	1064.52	Joback Method

cpg	711.75	J/mol×K	1104.43	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C493743&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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