3,5-Cyclohexadiene-1,2-dione, 3,5-bis(1,1-dimethylethyl)-

Other names: 3,5-Di-tert-butyl-o-quinone
3,5-bis(1,1-dimethylethyl)-3,5-cyclohexadiene-1,2-dione
3,5-di-t-Butyl-o-benzoquinone
3,5-di-tert-Butyl-ortho-benzoquinone
3,5-di-tert-butyl-1,2-benzoquinone
3,5-di-tert-butyl-o-benzoquinone
3,5-di-tert-butylcyclohexa-3,5-diene-1,2-dione
o-Benzoquinone, 3,5-di-tert-butyl-

Inchi: InChI=1S/C14H20O2/c1-13(2,3)9-7-10(14(4,5)6)12(16)11(15)8-9/h7-8H,1-6H3

InchiKey: NOUZOVBGCDDMSX-UHFFFAOYSA-N

Formula: C14H20O2

SMILES: CC(C)(C)C1=CC(=O)C(=O)C(C(C)(C)C)=C1

Mol. weight [g/mol]: 220.31

CAS: 3383-21-9

Physical Properties

Property code	Value	Unit	Source
ea	1.80 ± 0.09	eV	NIST Webbook
gf	-99.68	kJ/mol	Joback Method
hf	-457.91	kJ/mol	Joback Method
hfus	8.64	kJ/mol	Joback Method
hvap	55.31	kJ/mol	Joback Method
ie	8.81	eV	NIST Webbook
log10ws	-3.36		Crippen Method
logp	3.083		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
tb	681.40	K	Joback Method
tc	924.70	K	Joback Method
tf	388.50	K	Standard thermochemical characteristics of combustion and formation of 3,5-di-tert-butyl-o-benzoquinone and 3,6-di-tert-butyl-o-benzoquinone at T = 298.15 K
vc	0.718	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.79	J/mol×K	681.40	Joback Method
cpg	557.81	J/mol×K	721.95	Joback Method
cpg	575.45	J/mol×K	762.50	Joback Method
cpg	591.74	J/mol×K	803.05	Joback Method
cpg	606.71	J/mol×K	843.60	Joback Method
cpg	620.37	J/mol×K	884.15	Joback Method
cpg	632.77	J/mol×K	924.70	Joback Method
hfust	26.53	kJ/mol	387.90	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Standard thermochemical characteristics of combustion and formation of 3,5-di-tert-butyl-o-benzoquinone and 3,6-di-tert-butyl-O-benzoquinone at T = 298.15 K:	https://www.doi.org/10.1016/j.jct.2015.09.003
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=C3383219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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