2,5-di-tert-Butyl-1,4-benzoquinone

Other names:	2,5-di-tert-Butyl-p-quinone
	2,5-Cyclohexadiene-1,4-dione, 2,5-bis(1,1-dimethylethyl)-
	p-Benzoquinone, 2,5-di-tert-butyl-
	2,5-di-tert-Butylbenzoquinone
	2,5-Di-tert-butylquinone
	2,5-Di-tert-butylsemiquinone
	2,5-Ditert-butylbenzo-1,4-quinone
	2,5-Di-t-butyl-p-benzoquinone
	2,5-Di-tert-butyl-p-benzoquinone
	NSC 43579
	NSC 7489
Inchi:	InChI=1S/C14H20O2/c1-13(2,3)9-7-12(16)10(8-11(9)15)14(4,5)6/h7-8H,1-6H3
InchiKey:	ZZYASVWWDLJXIM-UHFFFAOYSA-N
Formula:	C14H20O2
SMILES:	CC(C)(C)C1=CC(=O)C(C(C)(C)C)=CC1=O
Mol. weight [g/mol]:	220.31
CAS:	2460-77-7

Physical Properties

Property code	Value	Unit	Source
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
log10ws	-3.36		Crippen Method
logp	3.083		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1466.00		NIST Webbook
rinpol	1466.00		NIST Webbook
tb	681.40	K	Joback Method
tc	924.70	K	Joback Method
tf	427.00	K	Joback Method
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

Sources

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=C2460777&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
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