tert-Butyl-p-benzoquinone

Other names:	2,5-Cyclohexadiene-1,4-dione, 2-(1,1-dimethylethyl)- p-Benzoquinone, 2-tert-butyl- tert-Butyl-1,4-benzoquinone tert-Butylbenzoquinone tert-Butylquinone 2-tert-Butyl-p-benzoquinone 2-tert-Butyl-1,4-benzoquinone 2-tert-Butyl quinone 2-tert-Butyl-p-quinone 2,5-Cyclohexadien-1,4-dione, 2-(1,1-dimethylethyl)- 2-(1,1-Dimethylethyl)-2,5-cyclohexadiene-1,4-dione NSC 124503 p-Benzoquinone, tert-butyl-
Inchi:	InChI=1S/C10H12O2/c1-10(2,3)8-6-7(11)4-5-9(8)12/h4-6H,1-3H3
InchiKey:	NCCTVAJNFXYWTM-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CC(C)(C)C1=CC(=O)C=CC1=O
Mol. weight [g/mol]:	164.20
CAS:	3602-55-9

Physical Properties

Property code	Value	Unit	Source
gf	-126.57	kJ/mol	Joback Method
hf	-355.13	kJ/mol	Joback Method
hfus	6.08	kJ/mol	Joback Method
hvap	47.04	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.667		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
ripol	2295.00		NIST Webbook
tb	588.13	K	Joback Method
tc	836.96	K	Joback Method
tf	366.98	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.21	J/mol×K	588.13	Joback Method
cpg	349.40	J/mol×K	629.60	Joback Method
cpg	364.58	J/mol×K	671.07	Joback Method
cpg	378.73	J/mol×K	712.55	Joback Method
cpg	391.84	J/mol×K	754.02	Joback Method
cpg	403.91	J/mol×K	795.49	Joback Method
cpg	414.92	J/mol×K	836.96	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=C3602559&Units=SI

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