2,5-CYCLOHEXADIENE-1,4-DIONE, 2,6-BIS(1,1-DIMETHYLETHYL)-

Other names: p-Benzoquinone, 2,6-di-tert-butyl-
2,6-Di-tert-butylbenzoquinone
2,6-Di-tert-butylquinone
2,6-di-tert-Butyl-para-benzoquinone
2,6-di-t-Butyl-p-benzoquinone
2,6-di-tert-Butyl-p-benzoquinone
2,6-Bis(1,1-Dimethylethyl)-2,5-cyclohexadiene-1,4-dione
DBQ
2,6-Di-tert-butyl-1,4-benzoquinone
2,6-bis-tert-Butylbenzoquinone
Benzoquinone, 2,6-di-(1,1-dimethylethyl)
p-Benzoquinone, 2,6-bis-(1,1-dimethylethyl)
NSC 14448
2,6-bis-(1,1-Dimethylethyl)-2,5-cycloxehadien-1,4-dione

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

InchiKey: RDQSIADLBQFVMY-UHFFFAOYSA-N

Formula: C14H20O2

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

Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
ea	1.87 ± 0.10	eV	NIST Webbook
hfus	8.64	kJ/mol	Joback Method
ie	9.29	eV	Cheméo Relay (1.0)
logp	3.083		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
rinpol	1458.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	1458.00		NIST Webbook
rinpol	1472.10		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1462.00		NIST Webbook

rinpol	1472.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1440.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1443.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1468.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1474.00		NIST Webbook
ripol	1809.00		NIST Webbook
ripol	1814.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1824.00		NIST Webbook
ripol	1809.00		NIST Webbook
tf	426.92	K	Cheméo Relay (1.0)

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: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C719222&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point