t-Butylhydroquinone

Other names:	1,4-Benzenediol, 2-(1,1-dimethylethyl)-
	Hydroquinone, tert-butyl-
	tert-Butyl-1,4-Benzenediol
	tert-Butylhydroquinone
	Mono-tert-butylhydroquinone
	MTBHQ
	TBHQ
	Mono-tertiarybutylhydroquinone
	2-tert-Butyl-1,4-benzenediol
	2-tert-Butylhydroquinone
	Sustane
	Tenox TBHQ
	2-t-Butyl-1,4-benzenediol
	2-(1,1-Dimethylethyl)-1,4-benzenediol
	Eastman MTBHQ
	2-t-Butylhydroquinone
	Banox 20BA
	NSC 4972
	2-tert-butyl-1,4-dihydroxybenzene
Inchi:	InChI=1S/C10H14O2/c1-10(2,3)8-6-7(11)4-5-9(8)12/h4-6,11-12H,1-3H3
InchiKey:	BGNXCDMCOKJUMV-UHFFFAOYSA-N
Formula:	C10H14O2
SMILES:	CC(C)(C)c1cc(O)ccc1O
Mol. weight [g/mol]:	166.22
CAS:	1948-33-0

Physical Properties

Property code	Value	Unit	Source
gf	-160.67	kJ/mol	Joback Method
hf	-376.57	kJ/mol	Joback Method
hfus	19.85	kJ/mol	Joback Method
hsub	104.40 ± 1.30	kJ/mol	NIST Webbook
hvap	64.86	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	2.395		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	4271.86	kPa	Joback Method

rinpol	1566.00		NIST Webbook
tb	612.89	K	Joback Method
tc	856.37	K	Joback Method
tf	454.74	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	364.71	J/mol×K	612.89	Joback Method
cpg	377.38	J/mol×K	653.47	Joback Method
cpg	389.01	J/mol×K	694.05	Joback Method
cpg	399.81	J/mol×K	734.63	Joback Method
cpg	409.96	J/mol×K	775.21	Joback Method
cpg	419.64	J/mol×K	815.79	Joback Method
cpg	429.06	J/mol×K	856.37	Joback Method
dvisc	0.0000897	Pa×s	481.10	Joback Method
dvisc	0.0001976	Pa×s	454.74	Joback Method
dvisc	0.0000442	Pa×s	507.46	Joback Method
dvisc	0.0000234	Pa×s	533.82	Joback Method
dvisc	0.0000131	Pa×s	560.17	Joback Method
dvisc	0.0000078	Pa×s	586.53	Joback Method
dvisc	0.0000048	Pa×s	612.89	Joback Method
hfust	27.74	kJ/mol	350.90	NIST Webbook
hsubt	101.20 ± 1.30	kJ/mol	350.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1948330&Units=SI

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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
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