tert-Butylhydroquinone, diacetate

Inchi: InChI=1S/C14H18O4/c1-9(15)17-11-6-7-13(18-10(2)16)12(8-11)14(3,4)5/h6-8H,1-5H3
InchiKey: SJRALGDWZXRRKL-UHFFFAOYSA-N
Formula: C14H18O4
SMILES: CC(=O)Oc1ccc(OC(C)=O)c(C(C)(C)C)c1
Mol. weight [g/mol]: 250.29

Physical Properties

Property code	Value	Unit	Source
gf	-304.85	kJ/mol	Joback Method
hf	-617.05	kJ/mol	Joback Method
hfus	23.44	kJ/mol	Joback Method
hvap	67.37	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.835		Crippen Method
mcvol	199.240	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	1695.10		NIST Webbook
tb	705.71	K	Joback Method
tc	922.82	K	Joback Method
tf	445.74	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.74	J/mol×K	705.71	Joback Method
cpg	556.41	J/mol×K	741.90	Joback Method
cpg	570.09	J/mol×K	778.08	Joback Method
cpg	582.79	J/mol×K	814.27	Joback Method
cpg	594.55	J/mol×K	850.45	Joback Method
cpg	605.37	J/mol×K	886.64	Joback Method
cpg	615.29	J/mol×K	922.82	Joback Method
dvisc	0.0008100	Pa×s	445.74	Joback Method
dvisc	0.0004893	Pa×s	489.07	Joback Method

dvisc	0.0003208	Pa×s	532.40	Joback Method
dvisc	0.0002241	Pa×s	575.73	Joback Method
dvisc	0.0001647	Pa×s	619.05	Joback Method
dvisc	0.0001259	Pa×s	662.38	Joback Method
dvisc	0.0000995	Pa×s	705.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352801&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

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
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