3-tert-Butyl-4-hydroxyanisole

Other names:	2-tert-Butyl-4-methoxyphenol
	Phenol, 2-(1,1-dimethylethyl)-4-methoxy-
	Phenol, 2-tert-butyl-4-methoxy-
	2-tert-Bha
	3-BHA
	4-Methoxy-2-tert-butylphenol
	4-Methoxy-6-tert-butylphenol
	o-tert-Butyl-p-methoxyphenol
	3-tert-Butyl-p-hydroxyanisole
	3-(1,1-Dimethylethyl)-4-hydroxyanisole
	2-(1,1-Dimethylethyl)-4-methoxyphenol
Inchi:	InChI=1S/C11H16O2/c1-11(2,3)9-7-8(13-4)5-6-10(9)12/h5-7,12H,1-4H3
InchiKey:	MRBKEAMVRSLQPH-UHFFFAOYSA-N
Formula:	C11H16O2
SMILES:	COc1ccc(O)c(C(C)(C)C)c1
Mol. weight [g/mol]:	180.24
CAS:	121-00-6

Physical Properties

Property code	Value	Unit	Source
gf	-112.26	kJ/mol	Joback Method
hf	-363.59	kJ/mol	Joback Method
hfus	17.46	kJ/mol	Joback Method
hvap	57.15	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.698		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	1497.00		NIST Webbook
rinpol	1496.00		NIST Webbook
tb	582.55	K	Joback Method
tc	809.07	K	Joback Method
tf	389.04	K	Joback Method
vc	0.516	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.74	J/mol×K	809.07	Joback Method
cpg	385.33	J/mol×K	582.55	Joback Method
cpg	400.12	J/mol×K	620.30	Joback Method
cpg	413.90	J/mol×K	658.06	Joback Method
cpg	426.77	J/mol×K	695.81	Joback Method
cpg	438.81	J/mol×K	733.56	Joback Method
cpg	450.10	J/mol×K	771.32	Joback Method
dvisc	0.0000295	Pa×s	582.55	Joback Method
dvisc	0.0010688	Pa×s	389.04	Joback Method
dvisc	0.0004674	Pa×s	421.29	Joback Method
dvisc	0.0002299	Pa×s	453.54	Joback Method
dvisc	0.0001242	Pa×s	485.79	Joback Method
dvisc	0.0000725	Pa×s	518.05	Joback Method
dvisc	0.0000451	Pa×s	550.30	Joback Method
hvapt	54.40	kJ/mol	433.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C121006&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
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature

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