Phenol, 3-(1,1-dimethylethyl)-4-methoxy-

Other names:	Phenol, 3-tert-butyl-4-methoxy-
	3-tert-Butylated hydroxyanisole
	3-tert-Butyl-4-methoxyphenol
	2-tert-Butyl-4-hydroxy anisole
	4-Methoxy-3-tert-butylphenol
Inchi:	InChI=1S/C11H16O2/c1-11(2,3)9-7-8(12)5-6-10(9)13-4/h5-7,12H,1-4H3
InchiKey:	IMOYOUMVYICGCA-UHFFFAOYSA-N
Formula:	C11H16O2
SMILES:	COc1ccc(O)cc1C(C)(C)C
Mol. weight [g/mol]:	180.24
CAS:	88-32-4

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	1490.00		NIST Webbook
rinpol	1490.00		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	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
cpg	460.74	J/mol×K	809.07	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
dvisc	0.0000295	Pa×s	582.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88324&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
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

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