Benzene, 1-(1,1-dimethylethoxy)-4-methoxy-

Other names:	Benzene, 1-tert-butoxy-4-methoxy- p-tert-butoxyanisole
Inchi:	InChI=1S/C11H16O2/c1-11(2,3)13-10-7-5-9(12-4)6-8-10/h5-8H,1-4H3
InchiKey:	SOEWHLJEXIKEPN-UHFFFAOYSA-N
Formula:	C11H16O2
SMILES:	COc1ccc(OC(C)(C)C)cc1
Mol. weight [g/mol]:	180.24
CAS:	15360-00-6

Physical Properties

Property code	Value	Unit	Source
gf	-62.64	kJ/mol	Joback Method
hf	-318.50	kJ/mol	Joback Method
hfus	12.86	kJ/mol	Joback Method
hvap	46.54	kJ/mol	Joback Method
ie	8.00 ± 0.01	eV	NIST Webbook
log10ws	-3.08		Crippen Method
logp	2.873		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2568.89	kPa	Joback Method
tb	524.35	K	Joback Method
tc	736.89	K	Joback Method
tf	299.55	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.49	J/mol×K	524.35	Joback Method
cpg	370.54	J/mol×K	559.77	Joback Method
cpg	385.71	J/mol×K	595.20	Joback Method
cpg	400.02	J/mol×K	630.62	Joback Method
cpg	413.50	J/mol×K	666.04	Joback Method
cpg	426.17	J/mol×K	701.47	Joback Method

cpg	438.05	J/mol×K	736.89	Joback Method
dvisc	0.0018734	Pa×s	299.55	Joback Method
dvisc	0.0009559	Pa×s	337.02	Joback Method
dvisc	0.0005580	Pa×s	374.48	Joback Method
dvisc	0.0003593	Pa×s	411.95	Joback Method
dvisc	0.0002489	Pa×s	449.42	Joback Method
dvisc	0.0001825	Pa×s	486.88	Joback Method
dvisc	0.0001399	Pa×s	524.35	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15360006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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