Benzene, 2-(1,1-dimethylethyl)-1,4-dimethoxy-

Other names:	Benzene, 2-tert-butyl-1,4-dimethoxy-
	3-t-Butyl-4-methoxyphenol methyl derivative
	1,4-Dimethoxy-2-tert-butylbenzene
	2-tert-Butyl-1,4-dimethoxybenzene
	tert-Butylhydroquinone, dimethyl ether
	Benzene, 1,4-dimethoxy-2-(1,1-dimethylethyl)
Inchi:	InChI=1S/C12H18O2/c1-12(2,3)10-8-9(13-4)6-7-11(10)14-5/h6-8H,1-5H3
InchiKey:	ALVJDUNBMKMTDC-UHFFFAOYSA-N
Formula:	C12H18O2
SMILES:	COc1ccc(OC)c(C(C)(C)C)c1
Mol. weight [g/mol]:	194.27
CAS:	21112-37-8

Physical Properties

Property code	Value	Unit	Source
gf	-63.85	kJ/mol	Joback Method
hf	-350.61	kJ/mol	Joback Method
hfus	15.06	kJ/mol	Joback Method
hvap	49.43	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	3.001		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	1425.40		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1408.00		NIST Webbook
ripol	1870.00		NIST Webbook
tb	552.21	K	Joback Method
tc	762.44	K	Joback Method
tf	323.34	K	Joback Method
vc	0.625	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.85	J/mol×K	552.21	Joback Method
cpg	475.86	J/mol×K	727.40	Joback Method
cpg	462.72	J/mol×K	692.36	Joback Method
cpg	448.77	J/mol×K	657.32	Joback Method
cpg	433.99	J/mol×K	622.29	Joback Method
cpg	418.35	J/mol×K	587.25	Joback Method
cpg	488.20	J/mol×K	762.44	Joback Method
dvisc	0.0001232	Pa×s	552.21	Joback Method
dvisc	0.0001581	Pa×s	514.07	Joback Method
dvisc	0.0002111	Pa×s	475.92	Joback Method
dvisc	0.0002966	Pa×s	437.78	Joback Method
dvisc	0.0004445	Pa×s	399.63	Joback Method
dvisc	0.0007257	Pa×s	361.49	Joback Method
dvisc	0.0013298	Pa×s	323.34	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21112378&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume