Benzene, (1,1-dimethylethoxy)-

Other names:	Ether, tert-butyl phenyl
	tert-Butoxybenzene
	tert-Butyl phenyl ether
	t-Butoxybenzene
	(1,1-Dimethylethoxy)benzene
Inchi:	InChI=1S/C10H14O/c1-10(2,3)11-9-7-5-4-6-8-9/h4-8H,1-3H3
InchiKey:	PNKZBZPLRKCVLI-UHFFFAOYSA-N
Formula:	C10H14O
SMILES:	CC(C)(C)Oc1ccccc1
Mol. weight [g/mol]:	150.22
CAS:	6669-13-2

Physical Properties

Property code	Value	Unit	Source
gf	43.57	kJ/mol	Joback Method
hf	-154.17	kJ/mol	Joback Method
hfus	9.47	kJ/mol	Joback Method
hvap	41.24	kJ/mol	Joback Method
ie	8.77	eV	NIST Webbook
ie	8.66	eV	NIST Webbook
ie	8.75	eV	NIST Webbook
log10ws	-2.96		Crippen Method
logp	2.864		Crippen Method
mcvol	133.870	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	1074.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1336.00		NIST Webbook
tb	465.15 ± 3.00	K	NIST Webbook
tb	471.15 ± 5.00	K	NIST Webbook
tc	690.87	K	Joback Method
tf	254.84 ± 0.30	K	NIST Webbook
vc	0.494	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	283.83	J/mol×K	474.07	Joback Method
cpg	299.88	J/mol×K	510.20	Joback Method
cpg	314.94	J/mol×K	546.34	Joback Method
cpg	329.04	J/mol×K	582.47	Joback Method
cpg	342.23	J/mol×K	618.60	Joback Method
cpg	354.55	J/mol×K	654.73	Joback Method
cpg	366.04	J/mol×K	690.87	Joback Method
dvisc	0.0039926	Pa×s	253.53	Joback Method
dvisc	0.0017530	Pa×s	290.29	Joback Method
dvisc	0.0009261	Pa×s	327.04	Joback Method
dvisc	0.0005566	Pa×s	363.80	Joback Method
dvisc	0.0003673	Pa×s	400.56	Joback Method
dvisc	0.0002599	Pa×s	437.31	Joback Method
dvisc	0.0001940	Pa×s	474.07	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6669132&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
ie: Ionization energy
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