4-tert-Butyltoluene

Other names:	1-(1,1-Dimethylethyl)-4-methyl-benzene
	1-(1,1-dimethylethyl)-4-methylbenzene
	1-Methyl-4-tert-butylbenzene
	1-methyl-4-(1,1-dimethylethyl)benzene
	1-tert-Butyl-4-Methylbenzene
	4-Methyl-tert-butylbenzene
	4-t-Butyltoluene
	4-tert-Butyl-1-Methylbenzene
	Benzene, 1-(1,1-dimethylethyl)-4-methyl-
	Benzene, 1-methyl-4-tert-butyl-
	NSC 6589
	TBT
	Toluene, p-tert-butyl-
	p-Methyl-tert-butylbenzene
	p-t-Butyl toluene
	p-tert-Butyltoluene
Inchi:	InChI=1S/C11H16/c1-9-5-7-10(8-6-9)11(2,3)4/h5-8H,1-4H3
InchiKey:	QCWXDVFBZVHKLV-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	Cc1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	148.24
CAS:	98-51-1

Physical Properties

Property code	Value	Unit	Source
gf	147.36	kJ/mol	Joback Method
hf	-57.00 ± 2.00	kJ/mol	NIST Webbook
hfus	10.48	kJ/mol	Joback Method
hvap	52.20 ± 0.60	kJ/mol	NIST Webbook
hvap	52.20 ± 0.10	kJ/mol	NIST Webbook
ie	8.31	eV	NIST Webbook
ie	8.12	eV	NIST Webbook
ie	8.28 ± 0.02	eV	NIST Webbook
log10ws	-3.26		Crippen Method
logp	3.293		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method

rinpol	1076.00	NIST Webbook
rinpol	1088.00	NIST Webbook
rinpol	1066.00	NIST Webbook
rinpol	1087.00	NIST Webbook
rinpol	1076.00	NIST Webbook
rinpol	1081.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1095.91	NIST Webbook
rinpol	1093.17	NIST Webbook
rinpol	1089.21	NIST Webbook
rinpol	1079.53	NIST Webbook
rinpol	1077.11	NIST Webbook
rinpol	1076.00	NIST Webbook
rinpol	1079.00	NIST Webbook
rinpol	1079.50	NIST Webbook
rinpol	1101.00	NIST Webbook
rinpol	1072.50	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1073.37	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1078.00	NIST Webbook
rinpol	1091.95	NIST Webbook
rinpol	1076.00	NIST Webbook
rinpol	1072.00	NIST Webbook
rinpol	1072.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1092.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1072.30	NIST Webbook
rinpol	1074.70	NIST Webbook
rinpol	1084.60	NIST Webbook
rinpol	1091.30	NIST Webbook
rinpol	1097.30	NIST Webbook
rinpol	1072.30	NIST Webbook
rinpol	1074.70	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1072.20	NIST Webbook
rinpol	1075.60	NIST Webbook
rinpol	1069.11	NIST Webbook
rinpol	1094.00	NIST Webbook
ripol	1304.90	NIST Webbook
ripol	1355.10	NIST Webbook
ripol	1341.00	NIST Webbook

ripol	1341.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1379.00		NIST Webbook
ripol	1329.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1305.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1353.00		NIST Webbook
tb	463.70	K	NIST Webbook
tb	466.20	K	NIST Webbook
tb	466.00	K	NIST Webbook
tb	465.90 ± 0.50	K	NIST Webbook
tb	465.90 ± 0.20	K	NIST Webbook
tb	465.90 ± 0.20	K	NIST Webbook
tb	462.00 ± 3.00	K	NIST Webbook
tb	463.00 ± 4.00	K	NIST Webbook
tb	464.00 ± 5.00	K	NIST Webbook
tb	466.00 ± 4.00	K	NIST Webbook
tb	461.00 ± 6.00	K	NIST Webbook
tb	463.00 ± 3.00	K	NIST Webbook
tc	696.31	K	Joback Method
tf	255.09	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.53	J/mol×K	479.51	Joback Method
cpg	320.58	J/mol×K	515.64	Joback Method
cpg	336.56	J/mol×K	551.78	Joback Method
cpg	351.51	J/mol×K	587.91	Joback Method
cpg	365.49	J/mol×K	624.04	Joback Method
cpg	378.55	J/mol×K	660.18	Joback Method
cpg	390.76	J/mol×K	696.31	Joback Method
dvisc	0.0016745	Pa×s	292.49	Joback Method
dvisc	0.0036767	Pa×s	255.09	Joback Method
dvisc	0.0009115	Pa×s	329.90	Joback Method
dvisc	0.0005616	Pa×s	367.30	Joback Method
dvisc	0.0003784	Pa×s	404.70	Joback Method
dvisc	0.0002726	Pa×s	442.11	Joback Method
dvisc	0.0002067	Pa×s	479.51	Joback Method

hvapt	52.30 ± 0.50	kJ/mol	296.50	NIST Webbook
hvapt	49.10	kJ/mol	403.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39787e+01
Coeff. B	-3.67669e+03
Coeff. C	-7.31190e+01
Temperature range (K), min.	341.66
Temperature range (K), max.	497.32

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and Modeling of Solid Liquid Equilibrium of Para-tert-Butylbenzoic Acid in Acetic Acid + Water and Acetic Acid + Para-tert-Butyltoluene Binary Systems at Various Temperatures:	https://www.doi.org/10.1021/acs.jced.6b00464
Measurement and Modeling of Solubility of para-tert-Butylbenzoic Acid in Methanol + Water and Acetic Acid + Para-tert-Butyltoluene Binary Solvents at Different Temperatures:	https://www.doi.org/10.1021/acs.jced.6b00965
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=C98511&Units=SI

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
ie:	Ionization energy

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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