2-tert-Butyltoluene

Other names:	1-tert-Butyl-2-methylbenzene
	o-tert-Butyltoluene
	Benzene, 1-(1,1-dimethylethyl)-2-methyl-
	Toluene, o-tert-butyl-
	1-Methyl-2-tert-butylbenzene
	2-t-Butyltoluene
	o-t-Butyltoluene
Inchi:	InChI=1S/C11H16/c1-9-7-5-6-8-10(9)11(2,3)4/h5-8H,1-4H3
InchiKey:	AXHVNJGQOJFMHT-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	Cc1ccccc1C(C)(C)C
Mol. weight [g/mol]:	148.24
CAS:	1074-92-6

Physical Properties

Property code	Value	Unit	Source
gf	147.36	kJ/mol	Joback Method
hf	-33.00 ± 2.00	kJ/mol	NIST Webbook
hfus	10.48	kJ/mol	Joback Method
hvap	41.72	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.293		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
rinpol	1115.00		NIST Webbook
rinpol	1117.20		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1122.80		NIST Webbook
rinpol	1113.40		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1122.80		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1090.90		NIST Webbook
rinpol	1120.00		NIST Webbook
rinpol	1113.40		NIST Webbook
rinpol	1088.40		NIST Webbook
tb	473.00	K	NIST Webbook

tb	473.60 ± 0.20	K	NIST Webbook
tb	473.60 ± 0.20	K	NIST Webbook
tb	473.60 ± 0.50	K	NIST Webbook
tc	696.31	K	Joback Method
tf	222.83 ± 0.15	K	NIST Webbook
tf	222.83 ± 0.10	K	NIST Webbook
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	0.0036767	Pa×s	255.09	Joback Method
dvisc	0.0016745	Pa×s	292.49	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

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=C1074926&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
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