BENZENE, 1-(1,1-DIMETHYLETHYL)-2-METHYL-

Other names: 1-Methyl-2-tert-butylbenzene
1-tert-Butyl-2-methylbenzene
2-t-Butyltoluene
Benzene, 1-(1,1-dimethylethyl)-2-methyl-
Toluene, o-tert-butyl-
o-t-Butyltoluene
o-tert-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]: 148.25

Physical Properties

Property code	Value	Unit	Source
af	0.3295		Cheméo Relay (1.0)
gf	147.36	kJ/mol	Joback Method
hf	-43.34	kJ/mol	Cheméo Relay (1.0)
hfus	10.48	kJ/mol	Joback Method
hvap	50.74	kJ/mol	Cheméo Relay (1.0)
ie	8.35	eV	Cheméo Relay (1.0)
log10ws	-4.27		Cheméo Relay (1.0)
logp	3.293		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
tb	466.40	K	Cheméo Relay (1.0)
tc	667.13	K	Cheméo Relay (1.0)
tf	217.09	K	Cheméo Relay (1.0)
vc	0.516	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1074926&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

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