Benzene, 1-(1,1-dimethylethyl)-3-methyl-

Other names:	1-Methyl-3-tert-butylbenzene
	1-tert-Butyl-3-Methylbenzene
	3-tert-Butyltoluene
	Benzene, 1-methyl-3-(1,1-dimethylethyl)-
	Benzene, 1-methyl-3-(1,1-dimethylpropyl)
	Toluene, m-tert-butyl-
	benzene, 1(1,1-dimethylethyl)-3-meth
	m-tert-Butyltoluene
Inchi:	InChI=1S/C11H16/c1-9-6-5-7-10(8-9)11(2,3)4/h5-8H,1-4H3
InchiKey:	JTIAYWZZZOZUTK-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	Cc1cccc(C(C)(C)C)c1
Mol. weight [g/mol]:	148.24
CAS:	1075-38-3

Physical Properties

Property code	Value	Unit	Source
gf	147.36	kJ/mol	Joback Method
hf	-54.00 ± 2.00	kJ/mol	NIST Webbook
hfus	10.48	kJ/mol	Joback Method
hvap	51.30 ± 0.60	kJ/mol	NIST Webbook
hvap	51.10 ± 0.30	kJ/mol	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	1053.60		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1062.30		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1052.00		NIST Webbook
rinpol	1067.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1072.00		NIST Webbook
rinpol	1067.50		NIST Webbook

rinpol	1051.12		NIST Webbook
rinpol	1056.10		NIST Webbook
rinpol	1072.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1296.00		NIST Webbook
ripol	1343.00		NIST Webbook
ripol	1361.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1332.00		NIST Webbook
ripol	1330.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1322.00		NIST Webbook
tb	459.00 ± 6.00	K	NIST Webbook
tb	461.00 ± 3.00	K	NIST Webbook
tb	462.44 ± 0.20	K	NIST Webbook
tb	462.44 ± 0.20	K	NIST Webbook
tb	462.50 ± 0.50	K	NIST Webbook
tb	462.50	K	NIST Webbook
tc	696.31	K	Joback Method
tf	231.76 ± 0.10	K	NIST Webbook
tf	231.74 ± 0.04	K	NIST Webbook
tf	231.76 ± 0.15	K	NIST Webbook
tf	231.78 ± 0.04	K	NIST Webbook
tf	231.75 ± 0.05	K	NIST Webbook
tf	231.74 ± 0.07	K	NIST Webbook
tf	231.78 ± 0.03	K	NIST Webbook
tf	231.75 ± 0.04	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
hvapt	51.40 ± 0.60	kJ/mol	296.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40175e+01
Coeff. B	-3.68728e+03
Coeff. C	-7.01090e+01
Temperature range (K), min.	338.67
Temperature range (K), max.	493.64

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=C1075383&Units=SI

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

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
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