Benzene, 1-bromo-3-methyl-

Other names:	1-Bromo-3-methylbenzene
	3-BROMOTOLUENE
	3-Bromo-1-methylbenzene
	3-Methyl-1-bromobenzene
	3-Methylbromobenzene
	5-Bromotoluene
	M-METHYLBROMOBENZENE
	M-TOLYL BROMIDE
	Toluene, m-bromo-
	m-Bromotoluene
Inchi:	InChI=1S/C7H7Br/c1-6-3-2-4-7(8)5-6/h2-5H,1H3
InchiKey:	WJIFKOVZNJTSGO-UHFFFAOYSA-N
Formula:	C7H7Br
SMILES:	Cc1cccc(Br)c1
Mol. weight [g/mol]:	171.03
CAS:	591-17-3

Physical Properties

Property code	Value	Unit	Source
affp	782.00	kJ/mol	NIST Webbook
basg	752.50	kJ/mol	NIST Webbook
gf	125.16	kJ/mol	Joback Method
hf	63.58	kJ/mol	Joback Method
hfus	12.82	kJ/mol	Joback Method
hvap	40.55	kJ/mol	Joback Method
ie	8.77	eV	NIST Webbook
ie	8.60 ± 0.10	eV	NIST Webbook
ie	8.81 ± 0.02	eV	NIST Webbook
log10ws	-3.52		Aqueous Solubility Prediction Method
logp	2.758		Crippen Method
mcvol	103.230	ml/mol	McGowan Method
pc	4414.96	kPa	Joback Method
rinpol	169.00		NIST Webbook
rinpol	1018.70		NIST Webbook
rinpol	169.00		NIST Webbook
rinpol	1055.00		NIST Webbook

rinpol	1033.00		NIST Webbook
rinpol	1018.70		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1033.00		NIST Webbook
rinpol	1043.00		NIST Webbook
rinpol	1095.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1498.00		NIST Webbook
tb	456.90	K	NIST Webbook
tb	457.16 ± 0.25	K	NIST Webbook
tb	457.45 ± 0.40	K	NIST Webbook
tc	691.11	K	Joback Method
tf	234.75 ± 1.00	K	NIST Webbook
tf	233.22	K	Aqueous Solubility Prediction Method
tf	235.01 ± 0.06	K	NIST Webbook
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.84	J/mol×K	691.11	Joback Method
cpg	183.69	J/mol×K	496.33	Joback Method
cpg	193.39	J/mol×K	535.29	Joback Method
cpg	202.41	J/mol×K	574.24	Joback Method
cpg	210.80	J/mol×K	613.20	Joback Method
cpg	218.60	J/mol×K	652.15	Joback Method
cpg	173.28	J/mol×K	457.38	Joback Method
dvisc	0.0003720	Pa×s	425.72	Joback Method
dvisc	0.0004698	Pa×s	394.05	Joback Method
dvisc	0.0006180	Pa×s	362.38	Joback Method
dvisc	0.0008568	Pa×s	330.72	Joback Method
dvisc	0.0012729	Pa×s	299.06	Joback Method
dvisc	0.0003042	Pa×s	457.38	Joback Method
dvisc	0.0020771	Pa×s	267.39	Joback Method
hvapt	49.40	kJ/mol	310.50	NIST Webbook
hvapt	47.70	kJ/mol	404.00	NIST Webbook
hvapt	48.30	kJ/mol	372.00	NIST Webbook

pvap	0.03	kPa	279.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.04	kPa	282.50	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.04	kPa	284.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.04	kPa	284.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.05	kPa	287.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.03	kPa	278.30	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.07	kPa	290.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.07	kPa	290.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.08	kPa	293.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.09	kPa	293.60	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.10	kPa	296.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.10	kPa	296.70	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.12	kPa	299.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.13	kPa	299.80	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.15	kPa	302.20	Thermochemistry of Halogen-Substituted Methylbenzenes

pvap	0.15	kPa	302.80	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.18	kPa	305.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.21	kPa	308.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.21	kPa	308.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.21	kPa	308.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.03	kPa	278.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.02	kPa	276.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.02	kPa	274.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.04	kPa	282.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.04	kPa	281.30	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.03	kPa	280.30	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.05	kPa	287.30	Thermochemistry of Halogen-Substituted Methylbenzenes

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40399e+01
Coeff. B	-3.66259e+03
Coeff. C	-6.81540e+01
Temperature range (K), min.	334.48
Temperature range (K), max.	487.77

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.85536e+02
Coeff. B	-1.67231e+04
Coeff. C	-4.10880e+01
Coeff. D	3.57145e-05
Temperature range (K), min.	314.15
Temperature range (K), max.	384.15

Sources

Thermochemistry of Halogen-Substituted Methylbenzenes: https://www.doi.org/10.1021/je500784s

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1699.mol

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C591173&Units=SI

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1699

Legend

affp: Proton affinity

basg: Gas basicity

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