Benzene, 1-bromo-4-methyl-

Other names:	1-Bromo-4-methylbenzene
	1-Methyl-4-bromobenzene
	4-BROMOTOLUENE
	4-Bromo-1-methylbenzene
	4-Methyl-1-bromobenzene
	4-Methylbromobenzene
	4-Methylphenyl bromide
	4-Tolyl bromide
	NSC 6531
	P-METHYLBROMOBENZENE
	P-TOLYL BROMIDE
	Parabromotoluene
	Toluene, p-bromo-
	p-Bromotoluene
	p-Methylphenyl bromide
	toluene, 4-bromo-
Inchi:	InChI=1S/C7H7Br/c1-6-2-4-7(8)5-3-6/h2-5H,1H3
InchiKey:	ZBTMRBYMKUEVEU-UHFFFAOYSA-N
Formula:	C7H7Br
SMILES:	Cc1ccc(Br)cc1
Mol. weight [g/mol]:	171.03
CAS:	106-38-7

Physical Properties

Property code	Value	Unit	Source
affp	775.30	kJ/mol	NIST Webbook
basg	745.80	kJ/mol	NIST Webbook
gf	125.16	kJ/mol	Joback Method
hf	63.58	kJ/mol	Joback Method
hfl	12.00	kJ/mol	NIST Webbook
hfus	12.82	kJ/mol	Joback Method
hvap	40.55	kJ/mol	Joback Method
ie	8.76	eV	NIST Webbook
ie	8.70 ± 0.10	eV	NIST Webbook
ie	8.71	eV	NIST Webbook
ie	8.67	eV	NIST Webbook
ie	8.68 ± 0.02	eV	NIST Webbook

ie	8.67 ± 0.02	eV	NIST Webbook
ie	8.68 ± 0.01	eV	NIST Webbook
ie	8.42	eV	NIST Webbook
log10ws	-3.19		Estimated Solubility Method
log10ws	-3.19		Aqueous Solubility Prediction Method
logp	2.758		Crippen Method
mcvol	103.230	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=2)		KDB
pc	4414.96	kPa	Joback Method
rinpol	1042.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1096.30		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	170.00		NIST Webbook
rinpol	1042.00		NIST Webbook
ripol	1493.00		NIST Webbook
tb	458.15	K	KDB
tb	457.50	K	NIST Webbook
tb	457.70 ± 0.50	K	NIST Webbook
tb	456.95 ± 0.50	K	NIST Webbook
tb	456.15 ± 2.00	K	NIST Webbook
tc	691.11	K	Joback Method
tf	301.00 ± 1.20	K	NIST Webbook
tf	298.00 ± 0.02	K	NIST Webbook
tf	299.73 ± 0.06	K	NIST Webbook
tf	301.30	K	Thermochemistry of Halogen-Substituted Methylbenzenes
tf	300.65	K	Aqueous Solubility Prediction Method
tf	299.85	K	KDB
tf	299.95 ± 1.00	K	NIST Webbook
tf	300.00 ± 1.50	K	NIST Webbook
tf	300.15 ± 1.50	K	NIST Webbook
tf	301.15 ± 0.60	K	NIST Webbook
tf	301.00 ± 1.20	K	NIST Webbook
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.28	J/mol×K	457.38	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	225.84	J/mol×K	691.11	Joback Method
dvisc	0.0003042	Pa×s	457.38	Joback Method
dvisc	0.0012729	Pa×s	299.06	Joback Method
dvisc	0.0020771	Pa×s	267.39	Joback Method
dvisc	0.0006180	Pa×s	362.38	Joback Method
dvisc	0.0004698	Pa×s	394.05	Joback Method
dvisc	0.0003720	Pa×s	425.72	Joback Method
dvisc	0.0008568	Pa×s	330.72	Joback Method
hfust	15.13	kJ/mol	301.20	NIST Webbook
hfust	15.13	kJ/mol	301.20	NIST Webbook
hvapt	47.10	kJ/mol	389.00	NIST Webbook
hvapt	55.30	kJ/mol	372.50	NIST Webbook
hvapt	45.80	kJ/mol	440.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40457e+01
Coeff. B	-3.66881e+03
Coeff. C	-6.83350e+01
Temperature range (K), min.	299.95
Temperature range (K), max.	488.38

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	3.29084e+01
Coeff. B	-6.26224e+03
Coeff. C	-2.39126e+00
Coeff. D	1.93939e-07
Temperature range (K), min.	299.95

Temperature range (K), max.	699.00

Sources

Thermochemistry of Halogen-Substituted Methylbenzenes:	https://www.doi.org/10.1021/je500784s
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1700.mol
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1700
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106387&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
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