Benzene, (bromomethyl)-

Other names:	(Bromomethyl)benzene
	1-Bromotoluene
	Benzyl bromide
	Bromophenylmethane
	Bromotoluene, «alpha»
	Bromotoluene, Â«alphaÂ»
	NSC 8041
	Phenylmethyl bromide
	Toluene, «alpha»-bromo-
	Toluene, Â«alphaÂ»-bromo-
	UN 1737
	«alpha»-Bromotoluene
	«omega»-Bromotoluene
	Â«alphaÂ»-Bromotoluene
	Â«omegaÂ»-Bromotoluene
Inchi:	InChI=1S/C7H7Br/c8-6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey:	AGEZXYOZHKGVCM-UHFFFAOYSA-N
Formula:	C7H7Br
SMILES:	BrCc1ccccc1
Mol. weight [g/mol]:	171.03
CAS:	100-39-0

Physical Properties

Property code	Value	Unit	Source
gf	134.79	kJ/mol	Joback Method
hf	84.00 ± 4.00	kJ/mol	NIST Webbook
hfl	16.00 ± 2.00	kJ/mol	NIST Webbook
hfl	22.00	kJ/mol	NIST Webbook
hfl	30.00 ± 14.00	kJ/mol	NIST Webbook
hfus	13.21	kJ/mol	Joback Method
hvap	53.70	kJ/mol	NIST Webbook
hvap	50.50 ± 0.50	kJ/mol	NIST Webbook
hvap	47.30 ± 4.20	kJ/mol	NIST Webbook
hvap	53.30 ± 0.70	kJ/mol	NIST Webbook
ie	9.10 ± 0.10	eV	NIST Webbook
ie	9.23	eV	NIST Webbook
ie	9.02 ± 0.02	eV	NIST Webbook

ie	8.99 ± 0.01	eV	NIST Webbook
ie	9.10 ± 0.05	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	8.99 ± 0.01	eV	NIST Webbook
log10ws	-2.78		Crippen Method
logp	2.582		Crippen Method
mcvol	103.230	ml/mol	McGowan Method
pc	4504.30	kPa	Joback Method
rinpol	1087.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1061.00		NIST Webbook
tb	471.00	K	NIST Webbook
tb	471.00	K	NIST Webbook
tb	471.70	K	NIST Webbook
tc	684.64	K	Joback Method
tf	271.75 ± 0.50	K	NIST Webbook
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	173.09	J/mol×K	452.40	Joback Method
cpg	184.03	J/mol×K	491.11	Joback Method
cpg	194.16	J/mol×K	529.81	Joback Method
cpg	203.55	J/mol×K	568.52	Joback Method
cpg	212.23	J/mol×K	607.23	Joback Method
cpg	220.26	J/mol×K	645.94	Joback Method
cpg	227.67	J/mol×K	684.64	Joback Method
dvisc	0.0010283	Pa×s	320.71	Joback Method
dvisc	0.0016279	Pa×s	287.79	Joback Method
dvisc	0.0029016	Pa×s	254.87	Joback Method
dvisc	0.0007076	Pa×s	353.63	Joback Method
dvisc	0.0005189	Pa×s	386.56	Joback Method
dvisc	0.0003995	Pa×s	419.48	Joback Method
dvisc	0.0003195	Pa×s	452.40	Joback Method
hfust	13.20	kJ/mol	271.80	NIST Webbook
hfust	13.20	kJ/mol	271.80	NIST Webbook
hvapt	46.90	kJ/mol	388.50	NIST Webbook
hvapt	48.10	kJ/mol	374.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.00	K	11.00	NIST Webbook
tbrp	400.00	K	11.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42835e+01
Coeff. B	-3.85387e+03
Coeff. C	-7.29640e+01
Temperature range (K), min.	348.32
Temperature range (K), max.	502.50

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C100390&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

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

Legend

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
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume