Benzene, (2-bromoethyl)-

Other names:	(2-Bromoethyl)benzene
	1-Bromo-2-phenylethane
	1-Phenyl-2-bromoethane
	2-Phenethyl bromide
	2-Phenyl-1-bromoethane
	2-Phenylethyl bromide
	NSC 33926
	Phenethyl bromide
	Phenylethyl bromide
	«beta»-Bromoethylbenzene
	«beta»-Phenethyl bromide
	«beta»-Phenylethyl bromide
	Â«betaÂ»-Bromoethylbenzene
	Â«betaÂ»-Phenethyl bromide
	Â«betaÂ»-Phenylethyl bromide
Inchi:	InChI=1S/C8H9Br/c9-7-6-8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey:	WMPPDTMATNBGJN-UHFFFAOYSA-N
Formula:	C8H9Br
SMILES:	BrCCc1ccccc1
Mol. weight [g/mol]:	185.06
CAS:	103-63-9

Physical Properties

Property code	Value	Unit	Source
gf	143.21	kJ/mol	Joback Method
hf	54.41	kJ/mol	Joback Method
hfus	15.80	kJ/mol	Joback Method
hvap	42.11	kJ/mol	Joback Method
ie	9.00 ± 0.10	eV	NIST Webbook
log10ws	-2.71		Crippen Method
logp	2.624		Crippen Method
mcvol	117.320	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
rinpol	1219.00		NIST Webbook
tb	493.70	K	NIST Webbook
tc	703.75	K	Joback Method
tf	217.22 ± 0.05	K	NIST Webbook

vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.89	J/mol×K	475.28	Joback Method
cpg	225.08	J/mol×K	513.36	Joback Method
cpg	236.43	J/mol×K	551.44	Joback Method
cpg	246.97	J/mol×K	589.51	Joback Method
cpg	256.76	J/mol×K	627.59	Joback Method
cpg	265.84	J/mol×K	665.67	Joback Method
cpg	274.27	J/mol×K	703.75	Joback Method
dvisc	0.0029592	Pa×s	266.14	Joback Method
dvisc	0.0016219	Pa×s	301.00	Joback Method
dvisc	0.0010071	Pa×s	335.85	Joback Method
dvisc	0.0006840	Pa×s	370.71	Joback Method
dvisc	0.0004965	Pa×s	405.57	Joback Method
dvisc	0.0003791	Pa×s	440.42	Joback Method
dvisc	0.0003012	Pa×s	475.28	Joback Method
hvapt	51.50	kJ/mol	374.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	490.70	K	97.90	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57301e+01
Coeff. B	-4.39729e+03
Coeff. C	-7.79680e+01
Temperature range (K), min.	362.72

Temperature range (K), max.	500.03

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103639&Units=SI

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
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