Benzene, (1-bromoethyl)-

Other names:	(1-Bromoethyl)benzene
	(«alpha»-Bromoethyl)benzene
	(Â«alphaÂ»-Bromoethyl)benzene
	1-Bromo-1-phenylethane
	1-Phenethyl bromide
	1-Phenyl-1-bromoethane
	1-Phenylethyl bromide
	NSC 8052
	«alpha»-Methylbenzyl bromide
	«alpha»-Phenethyl bromide
	«alpha»-Phenylethyl bromide
	Â«alphaÂ»-Methylbenzyl bromide
	Â«alphaÂ»-Phenethyl bromide
	Â«alphaÂ»-Phenylethyl bromide
Inchi:	InChI=1S/C8H9Br/c1-7(9)8-5-3-2-4-6-8/h2-7H,1H3
InchiKey:	CRRUGYDDEMGVDY-UHFFFAOYSA-N
Formula:	C8H9Br
SMILES:	CC(Br)c1ccccc1
Mol. weight [g/mol]:	185.06
CAS:	585-71-7

Physical Properties

Property code	Value	Unit	Source
gf	140.77	kJ/mol	Joback Method
hf	49.13	kJ/mol	Joback Method
hfus	12.28	kJ/mol	Joback Method
hvap	56.40 ± 0.30	kJ/mol	NIST Webbook
hvap	52.40	kJ/mol	NIST Webbook
log10ws	-3.16		Crippen Method
logp	3.143		Crippen Method
mcvol	117.320	ml/mol	McGowan Method
pc	4015.93	kPa	Joback Method
rinpol	1139.00		NIST Webbook
tb	474.84	K	Joback Method
tc	708.92	K	Joback Method
tf	251.14	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.09	J/mol×K	474.84	Joback Method
cpg	225.68	J/mol×K	513.85	Joback Method
cpg	237.36	J/mol×K	552.87	Joback Method
cpg	248.20	J/mol×K	591.88	Joback Method
cpg	258.23	J/mol×K	630.89	Joback Method
cpg	267.51	J/mol×K	669.90	Joback Method
cpg	276.09	J/mol×K	708.92	Joback Method
dvisc	0.0041027	Pa×s	251.14	Joback Method
dvisc	0.0019756	Pa×s	288.42	Joback Method
dvisc	0.0011246	Pa×s	325.71	Joback Method
dvisc	0.0007187	Pa×s	362.99	Joback Method
dvisc	0.0004993	Pa×s	400.27	Joback Method
dvisc	0.0003690	Pa×s	437.56	Joback Method
dvisc	0.0002860	Pa×s	474.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.20	K	2.10	NIST Webbook
tbrp	367.00	K	2.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	9.04032e+00
Coeff. B	-1.92124e+03
Coeff. C	-4.32180e+01
Temperature range (K), min.	222.70
Temperature range (K), max.	558.46

Sources

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=C585717&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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