Benzene, 1-bromo-4-ethenyl-

Other names:	Styrene, p-bromo- p-Bromostyrene 1-(4-Bromophenyl)ethylene 4-Bromostyrene 4-BrC6H4CH=CH2
Inchi:	InChI=1S/C8H7Br/c1-2-7-3-5-8(9)6-4-7/h2-6H,1H2
InchiKey:	WGGLDBIZIQMEGH-UHFFFAOYSA-N
Formula:	C8H7Br
SMILES:	C=Cc1ccc(Br)cc1
Mol. weight [g/mol]:	183.04
CAS:	2039-82-9

Physical Properties

Property code	Value	Unit	Source
affp	838.70	kJ/mol	NIST Webbook
basg	809.80	kJ/mol	NIST Webbook
gf	221.42	kJ/mol	Joback Method
hf	168.37	kJ/mol	Joback Method
hfus	14.13	kJ/mol	Joback Method
hvap	42.11	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.092		Crippen Method
mcvol	113.020	ml/mol	McGowan Method
pc	4114.41	kPa	Joback Method
tb	485.20	K	NIST Webbook
tc	712.22	K	Joback Method
tf	278.15 ± 2.00	K	NIST Webbook
vc	0.418	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.03	J/mol×K	673.00	Joback Method
cpg	250.42	J/mol×K	712.22	Joback Method

cpg	196.05	J/mol×K	476.94	Joback Method
cpg	206.94	J/mol×K	516.15	Joback Method
cpg	217.04	J/mol×K	555.37	Joback Method
cpg	226.38	J/mol×K	594.58	Joback Method
cpg	235.03	J/mol×K	633.79	Joback Method
dvisc	0.0002911	Pa×s	476.94	Joback Method
dvisc	0.0003553	Pa×s	443.60	Joback Method
dvisc	0.0019793	Pa×s	276.90	Joback Method
dvisc	0.0012112	Pa×s	310.24	Joback Method
dvisc	0.0008153	Pa×s	343.58	Joback Method
dvisc	0.0005886	Pa×s	376.92	Joback Method
dvisc	0.0004480	Pa×s	410.26	Joback Method
hvapt	49.90	kJ/mol	463.00	NIST Webbook
hvapt	48.50	kJ/mol	406.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.20	K	2.10	NIST Webbook

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=C2039829&Units=SI

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume