Benzene, (1-bromoethenyl)-

Other names:	Styrene, «alpha»-bromo-
	«alpha»-Bromostyrene
	1-Bromostyrene
	«alpha»-Bromostyrol
Inchi:	InChI=1S/C8H7Br/c1-7(9)8-5-3-2-4-6-8/h2-6H,1H2
InchiKey:	SRXJYTZCORKVNA-UHFFFAOYSA-N
Formula:	C8H7Br
SMILES:	C=C(Br)c1ccccc1
Mol. weight [g/mol]:	183.04
CAS:	98-81-7

Physical Properties

Property code	Value	Unit	Source
gf	222.50	kJ/mol	Joback Method
hf	170.05	kJ/mol	Joback Method
hfus	13.21	kJ/mol	Joback Method
hvap	41.52	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	3.052		Crippen Method
mcvol	113.020	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
tb	471.84	K	Joback Method
tc	710.60	K	Joback Method
tf	250.42	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.98	J/mol×K	471.84	Joback Method
cpg	207.56	J/mol×K	511.63	Joback Method
cpg	218.21	J/mol×K	551.43	Joback Method
cpg	228.02	J/mol×K	591.22	Joback Method
cpg	237.03	J/mol×K	631.01	Joback Method

cpg	245.31	J/mol×K	670.81	Joback Method
cpg	252.92	J/mol×K	710.60	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.70	K	0.50	NIST Webbook
tbrp	354.50 ± 1.50	K	1.30	NIST Webbook
tbrp	359.70	K	1.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98817&Units=SI
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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume