Benzene, (1,2-dibromoethyl)-

Other names:	(1,2-Dibromoethyl)benzene
	1,2-Dibromo-1-phenylethane
	1,2-Dibromo-2-phenylethane
	1,2-Dibromophenylethane
	1-Phenyl-1,2-dibromoethane
	Dowspray 9
	Styrene dibromide
	«alpha»,«beta»-Dibromoethylbenzene
	Â«alphaÂ»,Â«betaÂ»-Dibromoethylbenzene
Inchi:	InChI=1S/C8H8Br2/c9-6-8(10)7-4-2-1-3-5-7/h1-5,8H,6H2
InchiKey:	SHKKTLSDGJRCTR-UHFFFAOYSA-N
Formula:	C8H8Br2
SMILES:	BrCC(Br)c1ccccc1
Mol. weight [g/mol]:	263.96
CAS:	93-52-7

Physical Properties

Property code	Value	Unit	Source
gf	155.09	kJ/mol	Joback Method
hf	75.46	kJ/mol	Joback Method
hfus	17.56	kJ/mol	Joback Method
hvap	48.16	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.518		Crippen Method
mcvol	134.820	ml/mol	McGowan Method
pc	4391.59	kPa	Joback Method
tb	541.00	K	Joback Method
tc	791.67	K	Joback Method
tf	346.15 ± 3.00	K	NIST Webbook
tf	346.65 ± 1.50	K	NIST Webbook
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.46	J/mol×K	749.89	Joback Method
cpg	302.80	J/mol×K	791.67	Joback Method
cpg	247.25	J/mol×K	541.00	Joback Method
cpg	258.69	J/mol×K	582.78	Joback Method
cpg	269.15	J/mol×K	624.56	Joback Method
cpg	278.71	J/mol×K	666.34	Joback Method
cpg	287.46	J/mol×K	708.12	Joback Method
dvisc	0.0002854	Pa×s	541.00	Joback Method
dvisc	0.0003630	Pa×s	502.66	Joback Method
dvisc	0.0029370	Pa×s	310.94	Joback Method
dvisc	0.0016090	Pa×s	349.28	Joback Method
dvisc	0.0009929	Pa×s	387.63	Joback Method
dvisc	0.0006683	Pa×s	425.97	Joback Method
dvisc	0.0004803	Pa×s	464.31	Joback Method
hvapt	64.90	kJ/mol	443.00	NIST Webbook
hvapt	50.80	kJ/mol	458.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43381e+01
Coeff. B	-4.32591e+03
Coeff. C	-9.02860e+01
Temperature range (K), min.	398.17
Temperature range (K), max.	569.52

Sources

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=C93527&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

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