Benzene, 1,2-bis(bromomethyl)-

Other names:	1,2-Bis(bromomethyl)benzene
	1,2-Di(bromomethyl)benzene
	o-(Bromomethyl)benzyl bromide
	o-Bis(bromomethyl)benzene
	o-Xylene, «alpha»,«alpha»'-dibromo-
	o-Xylene, Â«alphaÂ»,Â«alphaÂ»'-dibromo-
	o-Xylylene dibromide
	«alpha»,«alpha» '-Dibromo-ortho-xylene
	«alpha»,«alpha»'-Dibromo-o-xylene
	«alpha»,«alpha»'-Dibromo-o-xylol
	Â«alphaÂ»,Â«alphaÂ» '-Dibromo-ortho-xylene
	Â«alphaÂ»,Â«alphaÂ»'-Dibromo-o-xylene
	Â«alphaÂ»,Â«alphaÂ»'-Dibromo-o-xylol
Inchi:	InChI=1S/C8H8Br2/c9-5-7-3-1-2-4-8(7)6-10/h1-4H,5-6H2
InchiKey:	KGKAYWMGPDWLQZ-UHFFFAOYSA-N
Formula:	C8H8Br2
SMILES:	BrCc1ccccc1CBr
Mol. weight [g/mol]:	263.96
CAS:	91-13-4

Physical Properties

Property code	Value	Unit	Source
gf	147.90	kJ/mol	Joback Method
hf	69.27	kJ/mol	Joback Method
hfus	20.70	kJ/mol	Joback Method
hvap	49.21	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.476		Crippen Method
mcvol	134.820	ml/mol	McGowan Method
pc	4260.71	kPa	Joback Method
tb	546.42	K	Joback Method
tc	792.41	K	Joback Method
tf	368.00	K	NIST Webbook
tf	370.00 ± 1.00	K	NIST Webbook
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.05	J/mol×K	792.41	Joback Method
cpg	291.88	J/mol×K	751.41	Joback Method
cpg	284.13	J/mol×K	710.41	Joback Method
cpg	275.74	J/mol×K	669.41	Joback Method
cpg	266.63	J/mol×K	628.42	Joback Method
cpg	256.75	J/mol×K	587.42	Joback Method
cpg	246.03	J/mol×K	546.42	Joback Method
dvisc	0.0018157	Pa×s	338.46	Joback Method
dvisc	0.0002952	Pa×s	546.42	Joback Method
dvisc	0.0003607	Pa×s	511.76	Joback Method
dvisc	0.0004536	Pa×s	477.10	Joback Method
dvisc	0.0005914	Pa×s	442.44	Joback Method
dvisc	0.0008066	Pa×s	407.78	Joback Method
dvisc	0.0011654	Pa×s	373.12	Joback Method
hfust	26.78	kJ/mol	368.20	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	402.20	K	0.50	NIST Webbook
tbrp	402.00 ± 1.00	K	0.60	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

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=C91134&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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume