

# Benzene, 1,3-bis(bromomethyl)-

<b>Other names:</b>	1,3-Bis(bromomethyl)benzene NSC 28040 alpha,alpha'-Dibromo-m-xylene m-(Bromomethyl)benzyl bromide m-Bis(bromomethyl)benzene m-Xylene, «alpha», «alpha»'-dibromo- m-Xylene, Â«alphaÂ», Â«alphaÂ»'-dibromo- m-Xylylene dibromide m-«alpha», «alpha»'-Dibromoxylene m-Â«alphaÂ», Â«alphaÂ»'-Dibromoxylene «alpha», «alpha»'-Dibromo-1,3-xylene «alpha», «alpha»'-Dibromo-m-xylene «alpha», «alpha»'-Dibromo-meta-xylene «alpha», «alpha»'-m-Xylene dibromide Â«alphaÂ», Â«alphaÂ»'-Dibromo-1,3-xylene Â«alphaÂ», Â«alphaÂ»'-Dibromo-m-xylene Â«alphaÂ», Â«alphaÂ»'-Dibromo-meta-xylene Â«alphaÂ», Â«alphaÂ»'-m-Xylene dibromide
<b>Inchi:</b>	InChI=1S/C8H8Br2/c9-5-7-2-1-3-8(4-7)6-10/h1-4H,5-6H2
<b>InchiKey:</b>	OXHOPZLBSSTTBU-UHFFFAOYSA-N
<b>Formula:</b>	C8H8Br2
<b>SMILES:</b>	BrCc1cccc(CBr)c1
<b>Mol. weight [g/mol]:</b>	263.96
<b>CAS:</b>	626-15-3

## 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	350.00 ± 1.00	K	NIST Webbook
tf	350.00	K	NIST Webbook
vc	0.499	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	246.03	J/molxK	546.42	Joback Method
cpg	256.75	J/molxK	587.42	Joback Method
cpg	266.63	J/molxK	628.42	Joback Method
cpg	275.74	J/molxK	669.41	Joback Method
cpg	284.13	J/molxK	710.41	Joback Method
cpg	291.88	J/molxK	751.41	Joback Method
cpg	299.05	J/molxK	792.41	Joback Method
dvisc	0.0018157	Paxs	338.46	Joback Method
dvisc	0.0011654	Paxs	373.12	Joback Method
dvisc	0.0008066	Paxs	407.78	Joback Method
dvisc	0.0005914	Paxs	442.44	Joback Method
dvisc	0.0004536	Paxs	477.10	Joback Method
dvisc	0.0003607	Paxs	511.76	Joback Method
dvisc	0.0002952	Paxs	546.42	Joback Method
hfust	23.69	kJ/mol	350.20	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.70	K	2.70	NIST Webbook
tbrp	432.00 ± 1.00	K	1.60	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C626153&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C626153&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>pvap:</b>	Vapor pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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