

Benzene, 1,4-bis(bromomethyl)-

Other names:	1,4-Bis(bromomethyl)benzene 1,4-Dibromomethylbenzene NSC 6226 p-(Bromomethyl)benzene p-Bis(bromomethyl)benzene p-Xylene, «alpha»,«alpha»'-dibromo- p-Xylene, Â«alphaÂ»,Â«alphaÂ»'-dibromo- p-Xylylene bromide p-Xylylene dibromide p-«alpha»,«alpha»'-Dibromoxylene p-Â«alphaÂ»,Â«alphaÂ»'-Dibromoxylene «alpha»,«alpha»'-Dibromo-p-xylene Â«alphaÂ»,Â«alphaÂ»'-Dibromo-p-xylene
Inchi:	InChI=1S/C8H8Br2/c9-5-7-1-2-8(6-10)4-3-7/h1-4H,5-6H2
InchiKey:	RBZMSGOBSOCYHR-UHFFFAOYSA-N
Formula:	C8H8Br2
SMILES:	BrCc1ccc(CBr)cc1
Mol. weight [g/mol]:	263.96
CAS:	623-24-5

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	518.20	K	NIST Webbook
tb	518.00	K	NIST Webbook
tc	792.41	K	Joback Method
tf	419.00 ± 1.00	K	NIST Webbook
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	429.50 ± 1.50	K	1.45	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.39562e+01
Coeff. B	-4.04333e+03
Coeff. C	-8.51960e+01
Temperature range (K), min.	381.01
Temperature range (K), max.	552.92

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C623245&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	Ideal gas heat capacity
dv_{isc}:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log_{10ws}:	Log10 of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
p_{vap}:	Vapor pressure
t_b:	Normal Boiling Point Temperature
t_{brp}:	Boiling point at reduced pressure
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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