Benzene, hexabromo-

Other names:	Benzene hexabromide
	hexabromobenzene
	perbromobenzene
Inchi:	InChI=1S/C6Br6/c7-1-2(8)4(10)6(12)5(11)3(1)9
InchiKey:	CAYGQBVSOZLICD-UHFFFAOYSA-N
Formula:	C6Br6
SMILES:	Brc1c(Br)c(Br)c(Br)c(Br)c1Br
Mol. weight [g/mol]:	551.49
CAS:	87-82-1

Physical Properties

Property code	Value	Unit	Source
gf	149.82	kJ/mol	Joback Method
hf	169.99	kJ/mol	Joback Method
hfus	35.10	kJ/mol	Joback Method
hvap	73.15	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
log10ws	-8.45		Crippen Method
logp	6.262		Crippen Method
mcvol	176.640	ml/mol	McGowan Method
pc	7915.30	kPa	Joback Method
tb	785.22	K	Joback Method
tc	1096.09	K	Joback Method
tf	605.20	K	Joback Method
vc	0.635	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.14	J/mol×K	785.22	Joback Method
cpg	239.31	J/mol×K	837.03	Joback Method
cpg	242.43	J/mol×K	888.84	Joback Method
cpg	245.63	J/mol×K	940.66	Joback Method
cpg	249.05	J/mol×K	992.47	Joback Method

cpg	252.82	J/mol×K	1044.28	Joback Method
cpg	257.09	J/mol×K	1096.09	Joback Method
dvisc	0.0001772	Pa×s	785.22	Joback Method
dvisc	0.0003605	Pa×s	635.20	Joback Method
dvisc	0.0003048	Pa×s	665.21	Joback Method
dvisc	0.0004334	Pa×s	605.20	Joback Method
dvisc	0.0002272	Pa×s	725.21	Joback Method
dvisc	0.0001997	Pa×s	755.22	Joback Method
dvisc	0.0002615	Pa×s	695.21	Joback Method
hfust	24.60	kJ/mol	598.80	NIST Webbook
psub	2.33e-06	kPa	363.28	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	7.39e-06	kPa	373.39	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	1.78e-05	kPa	383.22	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	4.48e-05	kPa	392.95	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures
psub	1.16e-04	kPa	402.92	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures

psub	2.55e-04	kPa	412.93	Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement of Vapor Pressures of Selected PBDEs, Hexabromobenzene, and 1,2-Bis(2,4,6-tribromophenoxy)ethane at Elevated Temperatures:	https://www.doi.org/10.1021/je400520e
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=C87821&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume