Benzene, 1,4-dibromo-

Other names:	1,4-DIBROMOBENZENE
	Benzene, p-dibromo-
	p-Bromophenyl bromide
	p-Dibromobenzene
Inchi:	InChI=1S/C6H4Br2/c7-5-1-2-6(8)4-3-5/h1-4H
InchiKey:	SWJPEBQEEAHIGZ-UHFFFAOYSA-N
Formula:	C6H4Br2
SMILES:	Brc1ccc(Br)cc1
Mol. weight [g/mol]:	235.90
CAS:	106-37-6

Physical Properties

Property code	Value	Unit	Source
chs	-2942.11	kJ/mol	NIST Webbook
gf	131.06	kJ/mol	Joback Method
hf	110.55	kJ/mol	Joback Method
hfpi	979.00	kJ/mol	NIST Webbook
hfpiz	1000.00	kJ/mol	NIST Webbook
hfus	20.39	kJ/mol	Low-Temperature Heat Capacities and Derived Thermodynamic Functions of 1,4 Dichlorobenzene, 1,4 Dibromobenzene, 1,3,5 Trichlorobenzene, and 1,3,5 Tribromobenzene
hsub	59.80	kJ/mol	NIST Webbook
hsub	74.23 ± 0.11	kJ/mol	NIST Webbook
hvap	44.76	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
ie	8.90 ± 0.03	eV	NIST Webbook
ie	8.91	eV	NIST Webbook
ie	8.97	eV	NIST Webbook
ie	8.82 ± 0.03	eV	NIST Webbook
ie	8.82 ± 0.02	eV	NIST Webbook
ie	8.85 ± 0.02	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	8.90 ± 0.15	eV	NIST Webbook
ie	8.91	eV	NIST Webbook

log10ws	-4.07		Estimated Solubility Method
log10ws	-4.07		Aqueous and cosolvent solubility data for drug-like organic compounds
log10ws	-4.07		Aqueous Solubility Prediction Method
logp	3.212		Crippen Method
mcvol	106.640	ml/mol	McGowan Method
pc	5569.17	kPa	Joback Method
rinpol	1193.00		NIST Webbook
rinpol	1190.00		NIST Webbook
rinpol	1193.00		NIST Webbook
rinpol	1193.00		NIST Webbook
tb	493.40	K	KDB
tb	491.70	K	NIST Webbook
tb	493.40 ± 0.60	K	NIST Webbook
tb	493.55 ± 0.07	K	NIST Webbook
tb	493.40 ± 0.40	K	NIST Webbook
tc	757.23	K	Joback Method
tf	360.45	K	KDB
tf	360.81	K	Aqueous Solubility Prediction Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	192.30	J/mol×K	671.70	Joback Method
cpg	197.86	J/mol×K	714.47	Joback Method
cpg	163.98	J/mol×K	500.66	Joback Method
cpg	172.09	J/mol×K	543.42	Joback Method
cpg	179.47	J/mol×K	586.18	Joback Method
cpg	186.19	J/mol×K	628.94	Joback Method
cpg	202.93	J/mol×K	757.23	Joback Method
cps	145.60	J/mol×K	198.15	NIST Webbook
cps	174.50	J/mol×K	299.80	NIST Webbook
dvisc	0.0004259	Pa×s	469.87	Joback Method
dvisc	0.0003533	Pa×s	500.66	Joback Method
dvisc	0.0018711	Pa×s	315.92	Joback Method
dvisc	0.0012528	Pa×s	346.71	Joback Method
dvisc	0.0008955	Pa×s	377.50	Joback Method
dvisc	0.0006734	Pa×s	408.29	Joback Method

dvisc	0.0005270	Pa×s	439.08	Joback Method
hfust	20.04	kJ/mol	360.00	NIST Webbook
hfust	20.53	kJ/mol	360.05	NIST Webbook
hfust	20.39	kJ/mol	360.50	NIST Webbook
hfust	20.04	kJ/mol	360.10	NIST Webbook
hfust	20.04	kJ/mol	360.10	NIST Webbook
hsubt	73.30 ± 0.40	kJ/mol	315.50	NIST Webbook
hsubt	73.80	kJ/mol	287.50	NIST Webbook
hsubt	73.20	kJ/mol	326.00	NIST Webbook
hsubt	73.30 ± 0.40	kJ/mol	326.00	NIST Webbook
hvapt	49.90	kJ/mol	433.00	NIST Webbook
sfust	57.00	J/mol×K	360.05	NIST Webbook
sfust	55.70	J/mol×K	360.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38785e+01
Coeff. B	-3.83251e+03
Coeff. C	-7.78290e+01
Temperature range (K), min.	359.82
Temperature range (K), max.	525.19

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.17523e+01
Coeff. B	-8.20361e+03
Coeff. C	-6.65907e+00
Coeff. D	3.22167e-06
Temperature range (K), min.	373.15
Temperature range (K), max.	493.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1676.mol
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1676
Low-Temperature Heat Capacities and Derived Thermodynamic Functions of 1,4 Dichlorobenzene, 1,4 Dibromobenzene, 1,3,5 Trichlorobenzene, and 1,3,5 Tribromobenzene:	https://www.doi.org/10.1021/je049762q
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106376&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfpi:	Enthalpy of formation of positive ion at standard conditions
hfpiz:	Enthalpy of formation of positive ion at 0K
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume