1,1'-Biphenyl, 4-bromo-

Other names:	4-Biphenyl bromide
	4-Brom-biphenyl
	4-Bromo-1,1'-biphenyl
	4-Bromobiphenyl
	4-Bromodiphenyl
	Biphenyl, 4-bromo-
	p-Bromobiphenyl
	p-Bromodiphenyl
	p-Phenylbromobenzene
Inchi:	InChI=1S/C12H9Br/c13-12-8-6-11(7-9-12)10-4-2-1-3-5-10/h1-9H
InchiKey:	PKJBWOWQJHHAHG-UHFFFAOYSA-N
Formula:	C12H9Br
SMILES:	Brc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	233.10
CAS:	92-66-0

Physical Properties

Property code	Value	Unit	Source
chs	-6123.49	kJ/mol	NIST Webbook
gf	279.67	kJ/mol	Joback Method
hf	196.91	kJ/mol	Joback Method
hfus	19.81	kJ/mol	Joback Method
hvap	53.95	kJ/mol	Joback Method
ie	8.05 ± 0.02	eV	NIST Webbook
log10ws	-5.24		Crippen Method
logp	4.116		Crippen Method
mcvol	149.920	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	583.00	K	NIST Webbook
tb	583.20	K	NIST Webbook
tc	864.14	K	Joback Method
tf	362.20 ± 0.30	K	NIST Webbook
tf	362.15 ± 1.50	K	NIST Webbook
tf	364.80 ± 0.20	K	NIST Webbook
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.51	J/mol×K	864.14	Joback Method
cpg	375.61	J/mol×K	819.86	Joback Method
cpg	365.83	J/mol×K	775.58	Joback Method
cpg	355.07	J/mol×K	731.30	Joback Method
cpg	343.23	J/mol×K	687.02	Joback Method
cpg	330.21	J/mol×K	642.74	Joback Method
cpg	315.92	J/mol×K	598.46	Joback Method
dvisc	0.0016627	Pa×s	350.16	Joback Method
dvisc	0.0002114	Pa×s	598.46	Joback Method
dvisc	0.0002624	Pa×s	557.08	Joback Method
dvisc	0.0003371	Pa×s	515.69	Joback Method
dvisc	0.0004526	Pa×s	474.31	Joback Method
dvisc	0.0006428	Pa×s	432.93	Joback Method
dvisc	0.0009832	Pa×s	391.54	Joback Method
hvapt	62.20	kJ/mol	477.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56477e+01
Coeff. B	-6.21507e+03
Coeff. C	-1.96480e+01
Temperature range (K), min.	424.27
Temperature range (K), max.	620.94

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C92660&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

chs:	Standard solid enthalpy of combustion
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume