1,1'-Biphenyl, 4,4'-dibromo-

Other names:	4,4'-Dibromobiphenyl
	4,4'-Dibromodiphenyl
	4,4'-dibromo-1,1'-biphenyl
	4,4-Dibromobiphenyl
	Biphenyl, 4,4'-dibromo-
	p,p'-Dibromobiphenyl
Inchi:	InChI=1S/C12H8Br2/c13-11-5-1-9(2-6-11)10-3-7-12(14)8-4-10/h1-8H
InchiKey:	HQJQYILBCQPYBI-UHFFFAOYSA-N
Formula:	C12H8Br2
SMILES:	Brc1ccc(-c2ccc(Br)cc2)cc1
Mol. weight [g/mol]:	312.00
CAS:	92-86-4

Physical Properties

Property code	Value	Unit	Source
gf	284.36	kJ/mol	Joback Method
hf	211.77	kJ/mol	Joback Method
hfus	28.38	kJ/mol	Thermal, solid liquid equilibrium, crystallization, and microstructural studies of organic monotectic alloy: 4,4 -Dibromobiphenyl succinonitrile
hvap	61.05	kJ/mol	Joback Method
log10ws	-7.74		Aqueous Solubility Prediction Method
logp	4.879		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
pc	3906.25	kPa	Joback Method
tb	630.70	K	NIST Webbook
tc	948.64	K	Joback Method
tf	437.00 ± 3.00	K	NIST Webbook
tf	442.00 ± 3.00	K	NIST Webbook
tf	437.00 ± 3.00	K	NIST Webbook
tf	437.00 ± 3.00	K	NIST Webbook
tf	438.00 ± 3.00	K	NIST Webbook
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.29	J/mol×K	669.60	Joback Method
cpg	359.51	J/mol×K	716.11	Joback Method
cpg	370.57	J/mol×K	762.61	Joback Method
cpg	380.59	J/mol×K	809.12	Joback Method
cpg	389.70	J/mol×K	855.63	Joback Method
cpg	398.01	J/mol×K	902.14	Joback Method
cpg	405.64	J/mol×K	948.64	Joback Method
dvisc	0.0010809	Pa×s	422.48	Joback Method
dvisc	0.0007137	Pa×s	463.67	Joback Method
dvisc	0.0005042	Pa×s	504.85	Joback Method
dvisc	0.0003754	Pa×s	546.04	Joback Method
dvisc	0.0002913	Pa×s	587.23	Joback Method
dvisc	0.0002337	Pa×s	628.41	Joback Method
dvisc	0.0001927	Pa×s	669.60	Joback Method
hfust	28.38	kJ/mol	440.70	NIST Webbook

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C92864&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Thermal, solid liquid equilibrium, crystallization, and microstructural studies of organic monotectic alloy: 4,4 -Dibromobiphenyl succinonitrile: https://www.doi.org/10.1016/j.tca.2009.06.012

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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