

1,1'-Biphenyl, 2-bromo-

Other names:	2-Bromobiphenyl 2-Bromodiphenyl o-Bromobiphenyl Biphenyl, 2-bromo-
Inchi:	InChI=1S/C12H9Br/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h1-9H
InchiKey:	KTADSLDAUJLZGL-UHFFFAOYSA-N
Formula:	C12H9Br
SMILES:	Brc1cccc1-c1cccc1
Mol. weight [g/mol]:	233.10
CAS:	2052-07-5

Physical Properties

Property code	Value	Unit	Source
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
log10ws	-5.24		Crippen Method
logp	4.116		Crippen Method
mcvol	149.920	ml/mol	McGowan Method
pc	3655.35	kPa	Joback Method
tb	570.20	K	NIST Webbook
tb	570.00 ± 1.00	K	NIST Webbook
tc	864.14	K	Joback Method
tf	350.16	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.92	J/mol×K	598.46	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	384.51	J/mol×K	864.14	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
dvisc	0.0016627	Pa×s	350.16	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.00	K	0.30	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2052075&Units=SI
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

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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