1,1'-Biphenyl, 3-bromo-

Other names:	Biphenyl, 3-bromo- m-Bromobiphenyl 3-Bromobiphenyl 3-Bromo diphenyl
Inchi:	InChI=1S/C12H9Br/c13-12-8-4-7-11(9-12)10-5-2-1-3-6-10/h1-9H
InchiKey:	USYQKCQEVBFJRP-UHFFFAOYSA-N
Formula:	C12H9Br
SMILES:	Brc1cccc(-c2ccccc2)c1
Mol. weight [g/mol]:	233.10
CAS:	2113-57-7

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	573.00 ± 1.00	K	NIST Webbook
tb	573.20	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	376.70	K	0.03	NIST Webbook
tbrp	384.00	K	0.10	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C2113577&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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