

1,1'-Biphenyl, 4-bromo-4'-methyl-

Other names:	Biphenyl, 4-bromo-4'-methyl-
Inchi:	InChI=1S/C13H11Br/c1-10-2-4-11(5-3-10)12-6-8-13(14)9-7-12/h2-9H,1H3
InchiKey:	MYWLXURJXCISCT-UHFFFAOYSA-N
Formula:	C13H11Br
SMILES:	<chem>Cc1ccc(-c2ccc(Br)cc2)cc1</chem>
Mol. weight [g/mol]:	247.13
CAS:	50670-49-0

Physical Properties

Property code	Value	Unit	Source
gf	278.46	kJ/mol	Joback Method
hf	164.80	kJ/mol	Joback Method
hfus	22.02	kJ/mol	Joback Method
hvap	56.84	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.425		Crippen Method
mcvol	164.010	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
tb	626.32	K	Joback Method
tc	886.66	K	Joback Method
tf	403.00 ± 4.00	K	NIST Webbook
vc	0.610	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.47	J/mol×K	626.32	Joback Method
cpg	377.23	J/mol×K	669.71	Joback Method
cpg	390.77	J/mol×K	713.10	Joback Method
cpg	403.18	J/mol×K	756.49	Joback Method
cpg	414.54	J/mol×K	799.88	Joback Method
cpg	424.95	J/mol×K	843.27	Joback Method
cpg	434.49	J/mol×K	886.66	Joback Method
dvisc	0.0012974	Paxs	373.95	Joback Method

dvisc	0.0008010	Paxs	416.01	Joback Method
dvisc	0.0005403	Paxs	458.07	Joback Method
dvisc	0.0003894	Paxs	500.13	Joback Method
dvisc	0.0002953	Paxs	542.20	Joback Method
dvisc	0.0002330	Paxs	584.26	Joback Method
dvisc	0.0001898	Paxs	626.32	Joback Method

Sources

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=C50670490&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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