

Biphenyl, 4-(bromomethyl)-

Inchi:	InChI=1S/C13H11Br/c14-10-11-6-8-13(9-7-11)12-4-2-1-3-5-12/h1-9H,10H2
InchiKey:	HZQLUIZFUXNFHK-UHFFFAOYSA-N
Formula:	C13H11Br
SMILES:	BrCc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	247.13
CAS:	2567-29-5

Physical Properties

Property code	Value	Unit	Source
gf	288.09	kJ/mol	Joback Method
hf	176.27	kJ/mol	Joback Method
hfus	22.40	kJ/mol	Joback Method
hvap	56.18	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.248		Crippen Method
mcvol	164.010	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
tb	621.34	K	Joback Method
tc	880.69	K	Joback Method
tf	361.43	K	Joback Method
vc	0.610	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.44	J/molxK	621.34	Joback Method
cpg	378.47	J/molxK	664.56	Joback Method
cpg	392.22	J/molxK	707.79	Joback Method
cpg	404.78	J/molxK	751.01	Joback Method
cpg	416.25	J/molxK	794.24	Joback Method
cpg	426.73	J/molxK	837.46	Joback Method
cpg	436.32	J/molxK	880.69	Joback Method
dvisc	0.0016055	Paxs	361.43	Joback Method
dvisc	0.0009325	Paxs	404.75	Joback Method

dvisc	0.0006016	Paxs	448.07	Joback Method
dvisc	0.0004193	Paxs	491.38	Joback Method
dvisc	0.0003098	Paxs	534.70	Joback Method
dvisc	0.0002396	Paxs	578.02	Joback Method
dvisc	0.0001920	Paxs	621.34	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=C2567295&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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