

1,1'-Biphenyl, 4-iodo-

Other names:	Biphenyl, 4-iodo- p-Iodobiphenyl p-Phenyliodobenzene 4-Biphenyl iodide 4-Iodobiphenyl 4-Iododiphenyl 4-Iodo-1,1'-biphenyl
Inchi:	InChI=1S/C12H9I/c13-12-8-6-11(7-9-12)10-4-2-1-3-5-10/h1-9H
InchiKey:	NXYICUMSYKIABQ-UHFFFAOYSA-N
Formula:	C12H9I
SMILES:	Ic1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	280.10
CAS:	1591-31-7

Physical Properties

Property code	Value	Unit	Source
gf	323.47	kJ/mol	Joback Method
hf	247.45	kJ/mol	Joback Method
hfus	18.93	kJ/mol	Joback Method
hvap	56.89	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	3.958		Crippen Method
mcvol	158.240	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
tb	625.44	K	Joback Method
tc	909.17	K	Joback Method
tf	348.42	K	Joback Method
vc	0.580	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.29	J/mol×K	625.44	Joback Method
cpg	340.44	J/mol×K	672.73	Joback Method

cpg	353.21	J/mol×K	720.02	Joback Method
cpg	364.74	J/mol×K	767.30	Joback Method
cpg	375.14	J/mol×K	814.59	Joback Method
cpg	384.55	J/mol×K	861.88	Joback Method
cpg	393.09	J/mol×K	909.17	Joback Method
dvisc	0.0020828	Paxs	348.42	Joback Method
dvisc	0.0011336	Paxs	394.59	Joback Method
dvisc	0.0007009	Paxs	440.76	Joback Method
dvisc	0.0004747	Paxs	486.93	Joback Method
dvisc	0.0003439	Paxs	533.10	Joback Method
dvisc	0.0002623	Paxs	579.27	Joback Method
dvisc	0.0002083	Paxs	625.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1591317&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
mccvol:	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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