

Biphenyl, 4,4'-diiodo-

Other names:	1,1'-Biphenyl, 4,4'-diiodo- Biphenyl, 4,4'-diiodo 4,4'-diiodobiphenyl
Inchi:	InChI=1S/C12H8I2/c13-11-5-1-9(2-6-11)10-3-7-12(14)8-4-10/h1-8H
InchiKey:	GPYDMVZCPRONLW-UHFFFAOYSA-N
Formula:	C12H8I2
SMILES:	Ic1ccc(-c2ccc(I)cc2)cc1
Mol. weight [g/mol]:	406.00

Physical Properties

Property code	Value	Unit	Source
af	0.4235		Cheméo Relay (1.0)
gf	371.96	kJ/mol	Joback Method
hf	312.66	kJ/mol	Cheméo Relay (1.0)
hfus	22.95	kJ/mol	Joback Method
hvap	91.83	kJ/mol	Cheméo Relay (1.0)
ie	8.10	eV	Cheméo Relay (1.0)
log10ws	-7.15		Cheméo Relay (1.0)
logp	4.563		Crippen Method
mcvol	184.060	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
tb	655.24	K	Cheméo Relay (1.0)
tc	897.91	K	Cheméo Relay (1.0)
tf	452.77	K	Cheméo Relay (1.0)
vc	0.612	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.44	J/mol×K	723.56	Joback Method
cpg	375.17	J/mol×K	775.98	Joback Method
cpg	385.67	J/mol×K	828.40	Joback Method
cpg	395.11	J/mol×K	880.82	Joback Method
cpg	403.68	J/mol×K	933.24	Joback Method

cpg	411.57	J/mol×K	985.66	Joback Method
cpg	418.95	J/mol×K	1038.07	Joback Method
dvisc	0.0014121	Pa×s	419.00	Joback Method
dvisc	0.0008183	Pa×s	469.76	Joback Method
dvisc	0.0005275	Pa×s	520.52	Joback Method
dvisc	0.0003676	Pa×s	571.28	Joback Method
dvisc	0.0002717	Pa×s	622.04	Joback Method
dvisc	0.0002102	Pa×s	672.80	Joback Method
dvisc	0.0001686	Pa×s	723.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3001158&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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