4-BIPHENYLCARBONITRILE

Other names:	4-Biphenylcarboxylic acid nitrile
	4-Cyanobiphenyl
	[1,1'-Biphenyl]-4-carbonitrile
	p-Cyanobiphenyl
	4-Biphenylcarbonitrile
Inchi:	InChI=1S/C13H9N/c14-10-11-6-8-13(9-7-11)12-4-2-1-3-5-12/h1-9H
InchiKey:	BPMBNLJJRKCCRT-UHFFFAOYSA-N
Formula:	C13H9N
SMILES:	N#Cc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	179.22

Physical Properties

Property code	Value	Unit	Source
af	0.4626		Cheméo Relay (1.0)
gf	406.95	kJ/mol	Joback Method
hf	334.66	kJ/mol	Cheméo Relay (1.0)
hfus	18.63	kJ/mol	Joback Method
hvap	84.23	kJ/mol	Cheméo Relay (1.0)
ie	8.99	eV	Cheméo Relay (1.0)
log10ws	-4.21		Cheméo Relay (1.0)
logp	3.225		Crippen Method
mcvol	147.890	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
tb	601.50	K	Cheméo Relay (1.0)
tc	860.67	K	Cheméo Relay (1.0)
tf	356.84	K	Cheméo Relay (1.0)
vc	0.545	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.64	J/mol×K	657.26	Joback Method
cpg	362.73	J/mol×K	700.53	Joback Method
cpg	374.69	J/mol×K	743.81	Joback Method

cpg	385.59	J/mol×K	787.08	Joback Method
cpg	395.50	J/mol×K	830.36	Joback Method
cpg	404.51	J/mol×K	873.63	Joback Method
cpg	412.70	J/mol×K	916.91	Joback Method

Sources

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=C2920389&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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