

[1,1'-Biphenyl]-4,4'-dicarbonitrile

Other names:	4,4'-Biphenyldicarbonitrile 4,4'-Dicyanobiphenyl 4,4'-Dicyanodiphenyl 4,4'-Diphenyldicarbonitrile
Inchi:	InChI=1S/C14H8N2/c15-9-11-1-5-13(6-2-11)14-7-3-12(10-16)4-8-14/h1-8H
InchiKey:	KAXYYLCSSXFXKR-UHFFFAOYSA-N
Formula:	C14H8N2
SMILES:	<chem>N#Cc1ccc(-c2ccc(C#N)cc2)cc1</chem>
Mol. weight [g/mol]:	204.23
CAS:	1591-30-6

Physical Properties

Property code	Value	Unit	Source
gf	538.92	kJ/mol	Joback Method
hf	447.59	kJ/mol	Joback Method
hfus	22.33	kJ/mol	Joback Method
hvap	73.59	kJ/mol	Joback Method
ie	10.40	eV	NIST Webbook
log10ws	-4.78		Crippen Method
logp	3.097		Crippen Method
mcvol	163.360	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
tb	787.20	K	Joback Method
tc	1051.08	K	Joback Method
tf	455.40	K	Joback Method
vc	0.655	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.25	J/mol×K	787.20	Joback Method
cpg	420.45	J/mol×K	831.18	Joback Method
cpg	429.70	J/mol×K	875.16	Joback Method
cpg	438.07	J/mol×K	919.14	Joback Method

cpg	445.64	J/mol×K	963.12	Joback Method
cpg	452.49	J/mol×K	1007.10	Joback Method
cpg	458.68	J/mol×K	1051.08	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=C1591306&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
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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