

4-Hydroxy-4'-nitrobiphenyl

Inchi:	InChI=1S/C12H9NO3/c14-12-7-3-10(4-8-12)9-1-5-11(6-2-9)13(15)16/h1-8,14H
InchiKey:	ZNDJDQOECGBUNK-UHFFFAOYSA-N
Formula:	C12H9NO3
SMILES:	O=[N+]([O-])c1ccc(-c2ccc(O)cc2)cc1
Mol. weight [g/mol]:	215.20
CAS:	3916-44-7

Physical Properties

Property code	Value	Unit	Source
gf	146.28	kJ/mol	Joback Method
hf	-17.49	kJ/mol	Joback Method
hfus	31.67	kJ/mol	Joback Method
hvap	77.12	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	2.967		Crippen Method
mvol	155.710	ml/mol	McGowan Method
pc	4098.62	kPa	Joback Method
tb	764.76	K	Joback Method
tc	1045.41	K	Joback Method
tf	545.69	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.78	J/molxK	764.76	Joback Method
cpg	427.36	J/molxK	811.53	Joback Method
cpg	438.06	J/molxK	858.31	Joback Method
cpg	448.05	J/molxK	905.08	Joback Method
cpg	457.54	J/molxK	951.86	Joback Method
cpg	466.71	J/molxK	998.63	Joback Method
cpg	475.76	J/molxK	1045.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3916447&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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