4-Cyano-4'-hydroxybiphenyl

Inchi: InChI=1S/C13H9NO/c14-9-10-1-3-11(4-2-10)12-5-7-13(15)8-6-12/h1-8,15H
InchiKey: ZRMIETZFPZGBEB-UHFFFAOYSA-N
Formula: C13H9NO
SMILES: N#Cc1ccc(-c2ccc(O)cc2)cc1
Mol. weight [g/mol]: 195.22
CAS: 19812-93-2

Physical Properties

Property code	Value	Unit	Source
gf	252.33	kJ/mol	Joback Method
hf	137.51	kJ/mol	Joback Method
hfus	24.41	kJ/mol	Joback Method
hvap	73.24	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	2.931		Crippen Method
mcvol	153.760	ml/mol	McGowan Method
pc	3480.65	kPa	Joback Method
tb	737.88	K	Joback Method
tc	1003.98	K	Joback Method
tf	478.34	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	392.17	J/mol×K	737.88	Joback Method
cpg	403.27	J/mol×K	782.23	Joback Method
cpg	413.55	J/mol×K	826.58	Joback Method
cpg	423.17	J/mol×K	870.93	Joback Method
cpg	432.28	J/mol×K	915.28	Joback Method
cpg	441.03	J/mol×K	959.63	Joback Method
cpg	449.58	J/mol×K	1003.98	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19812932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume