[1,1'-Biphenyl]-4-carbonitrile, 4'-(pentyloxy)-

Other names: 4'-(pentyloxy)[1,1'-biphenyl]-4-carbonitrile
4'-pentoxy-4-cyanobiphenyl
Inchi: InChI=1S/C18H19NO/c1-2-3-4-13-20-18-11-9-17(10-12-18)16-7-5-15(14-19)6-8-16/h5-12
InchiKey: RDISTOCQRJJICR-UHFFFAOYSA-N
Formula: C18H19NO
SMILES: CCCCCOc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]: 265.35
CAS: 52364-71-3

Physical Properties

Property code	Value	Unit	Source
gf	334.42	kJ/mol	Joback Method
hf	67.93	kJ/mol	Joback Method
hfus	32.37	kJ/mol	Joback Method
hvap	74.43	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	4.794		Crippen Method
mcvol	224.210	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
tb	799.06	K	Joback Method
tc	1030.58	K	Joback Method
tf	457.72	K	Joback Method
tt	339.75	K	Anchoring transition driven by short range ordering in calamitic-discotic composites
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.90	J/mol×K	799.06	Joback Method
cpg	649.65	J/mol×K	837.65	Joback Method
cpg	663.26	J/mol×K	876.23	Joback Method
cpg	675.78	J/mol×K	914.82	Joback Method

cpg	687.26	J/mol×K	953.40	Joback Method
cpg	697.76	J/mol×K	991.99	Joback Method
cpg	707.31	J/mol×K	1030.58	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Anchoring transition driven by short range ordering in calamitic-discotic composites:	https://www.doi.org/10.1016/j.tca.2015.08.007
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=C52364713&Units=SI

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
tt:	Triple Point Temperature
vc:	Critical Volume