[1,1'-Biphenyl]-4-carbonitrile, 4'-pentyl-

Other names:	4'-n-pentyl-4-biphenylcarbonitrile
	4'-pentyl[1,1'-biphenyl]-4-carbonitrile
	4-cyano-4'-pentylbiphenyl
Inchi:	InChI=1S/C18H19N/c1-2-3-4-5-15-6-10-17(11-7-15)18-12-8-16(14-19)9-13-18/h6-13H,2-
InchiKey:	HHPCNRKYVYWYAU-UHFFFAOYSA-N
Formula:	C18H19N
SMILES:	CCCCCc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]:	249.35
CAS:	40817-08-1

Physical Properties

Property code	Value	Unit	Source
gf	439.42	kJ/mol	Joback Method
hf	200.15	kJ/mol	Joback Method
hfus	13.66	kJ/mol	A new approach to study interaction parameters in cyanobiphenyl liquid crystal binary systems
hvap	72.02	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	4.958		Crippen Method
mcvol	218.340	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
tb	776.64	K	Joback Method
tc	1010.95	K	Joback Method
tf	295.70 ± 0.20	K	NIST Webbook
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.09	J/mol×K	776.64	Joback Method
cpg	623.34	J/mol×K	815.69	Joback Method
cpg	637.46	J/mol×K	854.74	Joback Method
cpg	650.53	J/mol×K	893.79	Joback Method

cpg	662.62	J/mol×K	932.84	Joback Method
cpg	673.80	J/mol×K	971.90	Joback Method
cpg	684.13	J/mol×K	1010.95	Joback Method

Sources

Phase Behavior of Liquid Crystal + CO2 Mixtures:	https://www.doi.org/10.1021/je500124r
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=C40817081&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
A new approach to study interaction parameters in cyanobiphenyl liquid crystal binary systems:	https://www.doi.org/10.1016/j.jct.2014.08.010

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