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

Other names: 1,1'-Biphenyl, 4-cyano-4'-hexyl-
4'-hexyl[1,1'-biphenyl]-4-carbonitrile
Inchi: InChI=1S/C19H21N/c1-2-3-4-5-6-16-7-11-18(12-8-16)19-13-9-17(15-20)10-14-19/h7-14H
InchiKey: VADSDVGLFDVIMG-UHFFFAOYSA-N
Formula: C19H21N
SMILES: CCCCCCc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]: 263.38
CAS: 41122-70-7

Physical Properties

Property code	Value	Unit	Source
gf	447.84	kJ/mol	Joback Method
hf	179.51	kJ/mol	Joback Method
hfus	33.78	kJ/mol	Joback Method
hvap	74.24	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	5.348		Crippen Method
mcvol	232.430	ml/mol	McGowan Method
pc	1686.56	kPa	Joback Method
tb	799.52	K	Joback Method
tc	1030.04	K	Joback Method
tf	286.70 ± 0.20	K	NIST Webbook
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	663.52	J/mol×K	799.52	Joback Method
cpg	679.02	J/mol×K	837.94	Joback Method
cpg	693.40	J/mol×K	876.36	Joback Method
cpg	706.73	J/mol×K	914.78	Joback Method
cpg	719.08	J/mol×K	953.20	Joback Method
cpg	730.52	J/mol×K	991.62	Joback Method
cpg	741.13	J/mol×K	1030.04	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=C41122707&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