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

Other names: 4'-(hexyloxy)[1,1'-biphenyl]-4-carbonitrile
Inchi: InChI=1S/C19H21NO/c1-2-3-4-5-14-21-19-12-10-18(11-13-19)17-8-6-16(15-20)7-9-17/h
InchiKey: YUYXUPYNSOFWFV-UHFFFAOYSA-N
Formula: C19H21NO
SMILES: CCCCCCOc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]: 279.38
CAS: 41424-11-7

Physical Properties

Property code	Value	Unit	Source
gf	342.84	kJ/mol	Joback Method
hf	47.29	kJ/mol	Joback Method
hfus	34.96	kJ/mol	Joback Method
hvap	76.65	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	5.184		Crippen Method
mcvol	238.300	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
tb	821.94	K	Joback Method
tc	1050.14	K	Joback Method
tf	331.00 ± 1.00	K	NIST Webbook
vc	0.927	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.82	J/mol×K	821.94	Joback Method
cpg	705.79	J/mol×K	859.97	Joback Method
cpg	719.61	J/mol×K	898.01	Joback Method
cpg	732.33	J/mol×K	936.04	Joback Method
cpg	744.02	J/mol×K	974.08	Joback Method
cpg	754.70	J/mol×K	1012.11	Joback Method
cpg	764.45	J/mol×K	1050.14	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C41424117&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
vc:	Critical Volume