4'-HEXYLOXY-4-BIPHENYLCARBONITRILE

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

Physical Properties

Property code	Value	Unit	Source
hfus	34.96	kJ/mol	Joback Method
ie	8.38	eV	Cheméo Relay (1.0)
logp	5.184		Crippen Method
mcvol	238.300	ml/mol	McGowan Method
tb	682.51	K	Cheméo Relay (1.0)
tf	331.00 ± 1.00	K	NIST Webbook

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41424117&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point