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

Other names:	4-Cyano-4'-(octyloxy)-1,1'-biphenyl
	p-Cyano-p'-(octyloxy)biphenyl
	4'-(n-Octyloxy)-4-cyanobiphenyl
	4-Cyano-4'-octoxybiphenyl
	4-(Octyloxy)-4'-cyanobiphenyl
	4-Cyano-4'-(n-octyloxy)biphenyl
	4'-(Octyloxy)-4-cyanobiphenyl
	p-(Octyloxy)-p'-cyanobiphenyl
	4'-(Octyloxy)-4-biphenylcarbonitrile
	4-(4-Octyloxyphenyl)benzonitrile
	8OCB
	M 24
	M 24 (liquid crystal)
	4'-(octyloxy)[1,1'-biphenyl]-4-carbonitrile
	Octyloxycyanobiphenyl
Inchi:	InChI=1S/C21H25NO/c1-2-3-4-5-6-7-16-23-21-14-12-20(13-15-21)19-10-8-18(17-22)9-1
InchiKey:	GPGGNNIMKOVSAG-UHFFFAOYSA-N
Formula:	C21H25NO
SMILES:	CCCCCCCCOc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]:	307.43
CAS:	52364-73-5

Physical Properties

Property code	Value	Unit	Source
gf	359.68	kJ/mol	Joback Method
hf	6.01	kJ/mol	Joback Method
hfus	40.14	kJ/mol	Joback Method
hvap	81.10	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	5.965		Crippen Method
mcvol	266.480	ml/mol	McGowan Method
pc	1430.46	kPa	Joback Method
tb	867.70	K	Joback Method
tc	1091.14	K	Joback Method
tf	327.70 ± 0.20	K	NIST Webbook
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.36	J/mol×K	867.70	Joback Method
cpg	820.67	J/mol×K	904.94	Joback Method
cpg	834.81	J/mol×K	942.18	Joback Method
cpg	847.84	J/mol×K	979.42	Joback Method
cpg	859.82	J/mol×K	1016.66	Joback Method
cpg	870.80	J/mol×K	1053.90	Joback Method
cpg	880.84	J/mol×K	1091.14	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=C52364735&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