

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

Other names:	4'-(heptyloxy)-4-biphenylcarbonitrile 4'-(heptyloxy)[1,1'-biphenyl]-4-carbonitrile 4-cyano-4'-heptyloxybiphenyl
Inchi:	InChI=1S/C20H23NO/c1-2-3-4-5-6-15-22-20-13-11-19(12-14-20)18-9-7-17(16-21)8-10-1
InchiKey:	JPBFKTCKZLMJED-UHFFFAOYSA-N
Formula:	C20H23NO
SMILES:	CCCCCCCOC1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]:	293.40
CAS:	52364-72-4

Physical Properties

Property code	Value	Unit	Source
gf	351.26	kJ/mol	Joback Method
hf	26.65	kJ/mol	Joback Method
hfus	37.55	kJ/mol	Joback Method
hvap	78.88	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	5.574		Crippen Method
mcvol	252.390	ml/mol	McGowan Method
pc	1540.29	kPa	Joback Method
tb	844.82	K	Joback Method
tc	1070.32	K	Joback Method
tf	326.70 ± 0.20	K	NIST Webbook
vc	0.984	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.66	J/mol×K	844.82	Joback Method
cpg	762.81	J/mol×K	882.40	Joback Method
cpg	776.80	J/mol×K	919.99	Joback Method
cpg	789.70	J/mol×K	957.57	Joback Method
cpg	801.54	J/mol×K	995.15	Joback Method
cpg	812.39	J/mol×K	1032.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52364724&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Phase Behavior of Liquid Crystal + CO2 Mixtures:	https://www.doi.org/10.1021/je500124r
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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