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

Other names:	4'-heptyl-4-biphenylcarbonitrile
	4'-heptyl[1,1'-biphenyl]-4-carbonitrile
	4-cyano-4'-heptylbiphenyl
Inchi:	InChI=1S/C20H23N/c1-2-3-4-5-6-7-17-8-12-19(13-9-17)20-14-10-18(16-21)11-15-20/h8-
InchiKey:	ZGOWXOZNUNZPAV-UHFFFAOYSA-N
Formula:	C20H23N
SMILES:	CCCCCCCc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]:	277.40
CAS:	41122-71-8

Physical Properties

Property code	Value	Unit	Source
gf	456.26	kJ/mol	Joback Method
hf	158.87	kJ/mol	Joback Method
hfus	24.35	kJ/mol	A new approach to study interaction parameters in cyanobiphenyl liquid crystal binary systems
hvap	76.47	kJ/mol	Joback Method
log10ws	-7.32		Crippen Method
logp	5.738		Crippen Method
mcvol	246.520	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
tb	822.40	K	Joback Method
tc	1049.70	K	Joback Method
tf	301.70 ± 0.20	K	NIST Webbook
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	719.94	J/mol×K	822.40	Joback Method
cpg	735.65	J/mol×K	860.28	Joback Method
cpg	750.24	J/mol×K	898.17	Joback Method
cpg	763.79	J/mol×K	936.05	Joback Method

cpg	776.37	J/mol×K	973.93	Joback Method
cpg	788.05	J/mol×K	1011.81	Joback Method
cpg	798.89	J/mol×K	1049.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41122718&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
A new approach to study interaction parameters in cyanobiphenyl liquid crystal binary systems:	https://www.doi.org/10.1016/j.jct.2014.08.010
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