4'-HEPTYL-4-BIPHENYLCARBONITRILE

Other names: 4'-heptyl[1,1'-biphenyl]-4-carbonitrile
4-cyano-4'-heptylbiphenyl
[1,1'-biphenyl]-4-carbonitrile, 4'-heptyl-
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]: 277.41

Physical Properties

Property code	Value	Unit	Source
af	0.7557		Cheméo Relay (1.0)
hfus	24.35	kJ/mol	A new approach to study interaction parameters in cyanobiphenyl liquid crystal binary systems
hvap	109.61	kJ/mol	Cheméo Relay (1.0)
ie	8.90	eV	Cheméo Relay (1.0)
log10ws	-7.29		Cheméo Relay (1.0)
logp	5.738		Crippen Method
mcvol	246.520	ml/mol	McGowan Method
pc	1561.05	kPa	Joback Method
tb	682.33	K	Cheméo Relay (1.0)
tc	907.86	K	Cheméo Relay (1.0)
tf	301.70 ± 0.20	K	NIST Webbook
vc	0.915	m3/kmol	Cheméo Relay (1.0)

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

A new approach to study interaction parameters in cyanobiphenyl liquid crystal binary systems:	https://www.doi.org/10.1016/j.jct.2014.08.010
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41122718&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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