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

Other names:	4'-Undecyl-biphenyl-4-carbonitrile
	4-Cyano-4'-undecylbiphenyl
	4'-undecyl[1,1'-biphenyl]-4-carbonitrile
	Undecylcyanobiphenyl
Inchi:	InChI=1S/C24H31N/c1-2-3-4-5-6-7-8-9-10-11-21-12-16-23(17-13-21)24-18-14-22(20-25)
InchiKey:	YIJBPYUXIFSTAP-UHFFFAOYSA-N
Formula:	C24H31N
SMILES:	CCCCCCCCCCCc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]:	333.51
CAS:	65860-74-4

Physical Properties

Property code	Value	Unit	Source
gf	489.94	kJ/mol	Joback Method
hf	76.31	kJ/mol	Joback Method
hfus	46.73	kJ/mol	Joback Method
hvap	85.37	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	7.299		Crippen Method
mcvol	302.880	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
tb	913.92	K	Joback Method
tc	1134.80	K	Joback Method
tf	326.00 ± 2.00	K	NIST Webbook
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	954.24	J/mol×K	913.92	Joback Method
cpg	970.64	J/mol×K	950.73	Joback Method
cpg	985.93	J/mol×K	987.55	Joback Method
cpg	1000.18	J/mol×K	1024.36	Joback Method
cpg	1013.48	J/mol×K	1061.17	Joback Method

cpg	1025.91	J/mol×K	1097.99	Joback Method
cpg	1037.55	J/mol×K	1134.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65860744&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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