4'-Undecyl-biphenyl-4-carbonitrile

Other names:	4'-Undecyl-biphenyl-4-carbonitrile
	4'-undecyl[1,1'-biphenyl]-4-carbonitrile
	4-Cyano-4'-undecylbiphenyl
	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]:	333.52

Physical Properties

Property code	Value	Unit	Source
af	0.9219		Cheméo Relay (1.0)
hfus	46.73	kJ/mol	Joback Method
hvap	127.43	kJ/mol	Cheméo Relay (1.0)
ie	9.00	eV	Cheméo Relay (1.0)
log10ws	-8.41		Cheméo Relay (1.0)
logp	7.299		Crippen Method
mcvol	302.880	ml/mol	McGowan Method
pc	1176.85	kPa	Joback Method
tb	710.06	K	Cheméo Relay (1.0)
tc	937.40	K	Cheméo Relay (1.0)
tf	318.57	K	Cheméo Relay (1.0)
vc	1.136	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C65860744&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

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