4'-OCTYL-4-BIPHENYLCARBONITRILE

Other names: 4'-octyl[1,1'-biphenyl]-4-carbonitrile
Inchi: InChI=1S/C21H25N/c1-2-3-4-5-6-7-8-18-9-13-20(14-10-18)21-15-11-19(17-22)12-16-21/
InchiKey: CSQPODPWWMOTIY-UHFFFAOYSA-N
Formula: C21H25N
SMILES: CCCCCCCCc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]: 291.44

Physical Properties

Property code	Value	Unit	Source
af	0.7981		Cheméo Relay (1.0)
hfus	38.96	kJ/mol	Joback Method
hvap	113.88	kJ/mol	Cheméo Relay (1.0)
ie	8.92	eV	Cheméo Relay (1.0)
log10ws	-7.58		Cheméo Relay (1.0)
logp	6.128		Crippen Method
mcvol	260.610	ml/mol	McGowan Method
pc	1449.04	kPa	Joback Method
tb	689.64	K	Cheméo Relay (1.0)
tc	915.75	K	Cheméo Relay (1.0)
tf	294.00 ± 1.00	K	NIST Webbook
tt	294.80 ± 0.50	K	NIST Webbook
vc	0.971	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.27	J/mol×K	845.28	Joback Method
cpg	793.17	J/mol×K	882.73	Joback Method
cpg	807.95	J/mol×K	920.17	Joback Method
cpg	821.70	J/mol×K	957.62	Joback Method
cpg	834.47	J/mol×K	995.07	Joback Method
cpg	846.35	J/mol×K	1032.52	Joback Method
cpg	857.42	J/mol×K	1069.96	Joback Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52709849&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):	

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
tt:	Triple Point Temperature
vc:	Critical Volume