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

Other names: 4'-butyl[1,1'-biphenyl]-4-carbonitrile
Inchi: InChI=1S/C17H17N/c1-2-3-4-14-5-9-16(10-6-14)17-11-7-15(13-18)8-12-17/h5-12H,2-4H
InchiKey: PJPLBHHDTUICNN-UHFFFAOYSA-N
Formula: C17H17N
SMILES: CCCCc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]: 235.32
CAS: 52709-83-8

Physical Properties

Property code	Value	Unit	Source
gf	431.00	kJ/mol	Joback Method
hf	220.79	kJ/mol	Joback Method
hfus	28.60	kJ/mol	Joback Method
hvap	69.79	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	4.568		Crippen Method
mcvol	204.250	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
tb	753.76	K	Joback Method
tc	992.39	K	Joback Method
tf	319.70 ± 0.20	K	NIST Webbook
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.72	J/mol×K	753.76	Joback Method
cpg	568.66	J/mol×K	793.53	Joback Method
cpg	582.48	J/mol×K	833.30	Joback Method
cpg	595.24	J/mol×K	873.07	Joback Method
cpg	607.02	J/mol×K	912.85	Joback Method
cpg	617.88	J/mol×K	952.62	Joback Method
cpg	627.90	J/mol×K	992.39	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52709838&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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