Benzonitrile, 2-(4-methylphenyl)-

Other names:	2-(4-methylphenyl)benzonitrile
	2-(p-tolyl)benzonitrile
	2-(para-tolyl)benzonitrile
	2-Cyano-4'-methyl biphenyl
	2-cyano-4'-Methyl Biphenyl (OTBN)
	2-cyano-4'-methylbiphenyl
	4'-methyl-[1,1'-biphenyl]-2-carbonitrile
	4-methyl-2'-cyanobiphenyl
	[1,1'-Biphenyl]-2-carbonitrile, 4'-methyl-
Inchi:	InChI=1S/C14H11N/c1-11-6-8-12(9-7-11)14-5-3-2-4-13(14)10-15/h2-9H,1H3
InchiKey:	ZGQVZLSNEBEHFN-UHFFFAOYSA-N
Formula:	C14H11N
SMILES:	Cc1ccc(-c2ccccc2C#N)cc1
Mol. weight [g/mol]:	193.24
CAS:	114772-53-1

Physical Properties

Property code	Value	Unit	Source
gf	405.74	kJ/mol	Joback Method
hf	282.71	kJ/mol	Joback Method
hfus	20.83	kJ/mol	Joback Method
hvap	63.11	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	3.534		Crippen Method
mcvol	161.980	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
tb	685.12	K	Joback Method
tc	939.56	K	Joback Method
tf	324.55	K	Solid-liquid phase equilibrium and mixing properties of 2-Cyano-4'-methylbiphenyl in pure solvents
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.68	J/mol×K	685.12	Joback Method
cpg	411.24	J/mol×K	727.53	Joback Method
cpg	423.69	J/mol×K	769.93	Joback Method
cpg	435.10	J/mol×K	812.34	Joback Method
cpg	445.55	J/mol×K	854.75	Joback Method
cpg	455.10	J/mol×K	897.16	Joback Method
cpg	463.82	J/mol×K	939.56	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=C114772531&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solid-liquid phase equilibrium and mixing properties of 2-Cyano-4'-methylbiphenyl in pure solvents:	https://www.doi.org/10.1016/j.jct.2016.07.050

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