

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

Other names:	4'-Propylbiphenyl-4-carbonitrile 4'-propyl[1,1'-biphenyl]-4-carbonitrile
Inchi:	InChI=1S/C16H15N/c1-2-3-13-4-8-15(9-5-13)16-10-6-14(12-17)7-11-16/h4-11H,2-3H2,1H
InchiKey:	XFMPTZWVMVMELB-UHFFFAOYSA-N
Formula:	C16H15N
SMILES:	CCCC1CCC(-C2CCC(C#N)CC2)CC1
Mol. weight [g/mol]:	221.30
CAS:	58743-76-3

Physical Properties

Property code	Value	Unit	Source
gf	422.58	kJ/mol	Joback Method
hf	241.43	kJ/mol	Joback Method
hfus	26.01	kJ/mol	Joback Method
hvap	67.56	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.178		Crippen Method
mcvol	190.160	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
ss	324.77	J/mol×K	NIST Webbook
tb	730.88	K	Joback Method
tc	974.33	K	Joback Method
tf	339.00 ± 0.10	K	NIST Webbook
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.29	J/mol×K	893.18	Joback Method
cpg	562.78	J/mol×K	933.75	Joback Method
cpg	500.48	J/mol×K	730.88	Joback Method
cpg	515.05	J/mol×K	771.45	Joback Method
cpg	528.49	J/mol×K	812.03	Joback Method
cpg	540.88	J/mol×K	852.60	Joback Method

cpg	572.43	J/mol×K	974.33	Joback Method
cps	302.97	J/mol×K	298.15	NIST Webbook
hfust	22.70	kJ/mol	338.77	NIST Webbook
sfust	67.00	J/mol×K	338.77	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58743763&Units=SI

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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