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

Other names: 4'-propoxy[1,1'-biphenyl]-4-carbonitrile
Inchi: InChI=1S/C16H15NO/c1-2-11-18-16-9-7-15(8-10-16)14-5-3-13(12-17)4-6-14/h3-10H,2,1
InchiKey: RZCQJZFWJZHMPK-UHFFFAOYSA-N
Formula: C16H15NO
SMILES: CCCOc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]: 237.30
CAS: 52709-86-1

Physical Properties

Property code	Value	Unit	Source
gf	317.58	kJ/mol	Joback Method
hf	109.21	kJ/mol	Joback Method
hfus	27.19	kJ/mol	Joback Method
hvap	69.97	kJ/mol	Joback Method
log10ws	-5.38		Crippen Method
logp	4.014		Crippen Method
mcvol	196.030	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
tb	753.30	K	Joback Method
tc	993.10	K	Joback Method
tf	435.18	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.13	J/mol×K	753.30	Joback Method
cpg	540.27	J/mol×K	793.27	Joback Method
cpg	553.30	J/mol×K	833.23	Joback Method
cpg	565.25	J/mol×K	873.20	Joback Method
cpg	576.19	J/mol×K	913.17	Joback Method
cpg	586.14	J/mol×K	953.14	Joback Method
cpg	595.17	J/mol×K	993.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52709861&Units=SI
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

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