

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

Other names:	4'-ethyl[1,1'-biphenyl]-4-carbonitrile 4-ethyl-4'-cyanobiphenyl
Inchi:	InChI=1S/C15H13N/c1-2-12-3-7-14(8-4-12)15-9-5-13(11-16)6-10-15/h3-10H,2H2,1H3
InchiKey:	DLLIPJSMDJCZRF-UHFFFAOYSA-N
Formula:	C15H13N
SMILES:	CCc1ccc(-c2ccc(C#N)cc2)cc1
Mol. weight [g/mol]:	207.27
CAS:	58743-75-2

Physical Properties

Property code	Value	Unit	Source
gf	414.16	kJ/mol	Joback Method
hf	262.07	kJ/mol	Joback Method
hfus	23.42	kJ/mol	Joback Method
hvap	65.34	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	3.788		Crippen Method
mcvol	176.070	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
tb	708.00	K	Joback Method
tc	956.73	K	Joback Method
tf	401.68	K	Joback Method
vc	0.685	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.44	J/molxK	708.00	Joback Method
cpg	462.55	J/molxK	749.45	Joback Method
cpg	475.54	J/molxK	790.91	Joback Method
cpg	487.49	J/molxK	832.36	Joback Method
cpg	498.46	J/molxK	873.82	Joback Method
cpg	508.52	J/molxK	915.27	Joback Method
cpg	517.74	J/molxK	956.73	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=C58743752&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

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