

3,4'-Diisopropylbiphenyl

Other names:	1,1'-Biphenyl, 3,4'-bis-(1-methylethyl) 1,1'-Biphenyl, 3,4'-diisopropyl
Inchi:	InChI=1S/C18H22/c1-13(2)15-8-10-16(11-9-15)18-7-5-6-17(12-18)14(3)4/h5-14H,1-4H3
InchiKey:	LHNUPUGVRFQTLK-UHFFFAOYSA-N
Formula:	C18H22
SMILES:	CC(C)c1ccc(-c2cccc(C(C)C)c2)cc1
Mol. weight [g/mol]:	238.37
CAS:	61434-46-6

Physical Properties

Property code	Value	Unit	Source
gf	301.36	kJ/mol	Joback Method
hf	24.71	kJ/mol	Joback Method
hfus	22.63	kJ/mol	Joback Method
hvap	60.76	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.600		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinpol	1921.00		NIST Webbook
rinpol	1921.00		NIST Webbook
tb	673.68	K	Joback Method
tc	905.93	K	Joback Method
tf	340.50	K	Joback Method
vc	0.816	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.18	J/mol×K	673.68	Joback Method
cpg	597.85	J/mol×K	712.39	Joback Method
cpg	616.14	J/mol×K	751.10	Joback Method
cpg	633.14	J/mol×K	789.80	Joback Method
cpg	648.92	J/mol×K	828.51	Joback Method

cpg	663.54	J/mol×K	867.22	Joback Method
cpg	677.08	J/mol×K	905.93	Joback Method
dvisc	0.0020468	Pa×s	340.50	Joback Method
dvisc	0.0008817	Pa×s	396.03	Joback Method
dvisc	0.0004672	Pa×s	451.56	Joback Method
dvisc	0.0002845	Pa×s	507.09	Joback Method
dvisc	0.0001911	Pa×s	562.62	Joback Method
dvisc	0.0001378	Pa×s	618.15	Joback Method
dvisc	0.0001049	Pa×s	673.68	Joback Method

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=C61434466&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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