

1,1'-Biphenyl, 3,3'-diisopropyl

Inchi:	InChI=1S/C18H22/c1-13(2)15-7-5-9-17(11-15)18-10-6-8-16(12-18)14(3)4/h5-14H,1-4H3
InchiKey:	PYXYRWLLNHRLM-UHFFFAOYSA-N
Formula:	C18H22
SMILES:	CC(C)c1cccc(-c2cccc(C(C)C)c2)c1
Mol. weight [g/mol]:	238.37

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	1868.00		NIST Webbook
rinpol	1868.00		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/molxK	673.68	Joback Method
cpg	663.54	J/molxK	867.22	Joback Method
cpg	648.92	J/molxK	828.51	Joback Method
cpg	633.14	J/molxK	789.80	Joback Method
cpg	616.14	J/molxK	751.10	Joback Method
cpg	597.85	J/molxK	712.39	Joback Method
cpg	677.08	J/molxK	905.93	Joback Method
dvisc	0.0001049	Paxs	673.68	Joback Method

dvisc	0.0001378	Paxs	618.15	Joback Method
dvisc	0.0001911	Paxs	562.62	Joback Method
dvisc	0.0002845	Paxs	507.09	Joback Method
dvisc	0.0004672	Paxs	451.56	Joback Method
dvisc	0.0008817	Paxs	396.03	Joback Method
dvisc	0.0020468	Paxs	340.50	Joback Method

Sources

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=R11157&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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