

3,3'-Diisopropylbiphenyl

Other names:	3,3'-Diisopropylbiphenyl
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:	PYXYRWLLNHRM-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
af	0.5132		Cheméo Relay (1.0)
gf	301.36	kJ/mol	Joback Method
hf	17.27	kJ/mol	Cheméo Relay (1.0)
hfus	22.63	kJ/mol	Joback Method
hvap	89.29	kJ/mol	Cheméo Relay (1.0)
ie	8.08	eV	Cheméo Relay (1.0)
log10ws	-6.95		Cheméo Relay (1.0)
logp	5.600		Crippen Method
mcvol	216.960	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
tb	599.52	K	Cheméo Relay (1.0)
tc	820.17	K	Cheméo Relay (1.0)
tf	316.89	K	Cheméo Relay (1.0)
vc	0.806	m3/kmol	Cheméo Relay (1.0)

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

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C69375128&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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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