

1,1'-Biphenyl, 3-(1-methylethyl)-

Other names:	3-(1-Methylethyl)-1,1'-biphenyl 3-isopropylbiphenyl biphenyl, 3-isopropyl- m-isopropylbiphenyl
Inchi:	InChI=1S/C15H16/c1-12(2)14-9-6-10-15(11-14)13-7-4-3-5-8-13/h3-12H,1-2H3
InchiKey:	LIWRTHVZRZXVFX-UHFFFAOYSA-N
Formula:	C15H16
SMILES:	CC(C)c1cccc(-c2ccccc2)c1
Mol. weight [g/mol]:	196.29
CAS:	20282-30-8

Physical Properties

Property code	Value	Unit	Source
gf	288.17	kJ/mol	Joback Method
hf	103.38	kJ/mol	Joback Method
hfus	18.78	kJ/mol	Joback Method
hvap	53.81	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	4.477		Crippen Method
mcvol	174.690	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	1671.00		NIST Webbook
rinpol	277.70		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1660.00		NIST Webbook
ripol	2244.00		NIST Webbook
ripol	2204.00		NIST Webbook
ripol	2244.00		NIST Webbook
tb	566.54	K	Vapour pressures and enthalpies of vaporization of a series of the alkylbiphenyls
tc	841.46	K	Joback Method
tf	309.17	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.76	J/mol×K	600.50	Joback Method
cpg	440.19	J/mol×K	640.66	Joback Method
cpg	457.26	J/mol×K	680.82	Joback Method
cpg	473.06	J/mol×K	720.98	Joback Method
cpg	487.65	J/mol×K	761.14	Joback Method
cpg	501.11	J/mol×K	801.30	Joback Method
cpg	513.52	J/mol×K	841.46	Joback Method
dvisc	0.0024536	Pa×s	309.17	Joback Method
dvisc	0.0011250	Pa×s	357.73	Joback Method
dvisc	0.0006215	Pa×s	406.28	Joback Method
dvisc	0.0003897	Pa×s	454.84	Joback Method
dvisc	0.0002674	Pa×s	503.39	Joback Method
dvisc	0.0001960	Pa×s	551.95	Joback Method
dvisc	0.0001511	Pa×s	600.50	Joback Method

Sources

Vapour pressures and enthalpies of vaporization of a series of the anisole Method:

McGowan Method:

NIST Webbook:

Crippen Method:

Crippen Method:

<https://www.doi.org/10.1016/j.fluid.2012.08.020>

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

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

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C20282308&Units=SI>

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

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

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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