1,1'-Biphenyl, 3-methyl-

Other names: (3-Methylphenyl)benzene
1-methyl-3-phenylbenzene
3-Methyl-1,1'-biphenyl
3-Methylbiphenyl
3-Methyldiphenyl
3-Phenyltoluene
Biphenyl, 3-methyl-
m-Methylbiphenyl
m-Phenyltoluene

Inchi: InChI=1S/C13H12/c1-11-6-5-9-13(10-11)12-7-3-2-4-8-12/h2-10H,1H3

InchiKey: NPDIDUXTRAITDE-UHFFFAOYSA-N

Formula: C13H12

SMILES: Cc1cccc(-c2ccccc2)c1

Mol. weight [g/mol]: 168.23

CAS: 643-93-6

Physical Properties

Property code	Value	Unit	Source
affp	828.00	kJ/mol	NIST Webbook
basg	795.50	kJ/mol	NIST Webbook
chl	-6916.20 ± 7.10	kJ/mol	NIST Webbook
gf	273.77	kJ/mol	Joback Method
hf	149.94	kJ/mol	Joback Method
hfus	17.12	kJ/mol	Joback Method
hvap	69.60	kJ/mol	NIST Webbook
ie	7.95 ± 0.02	eV	NIST Webbook
log10ws	-4.55		Crippen Method
logp	3.662		Crippen Method
mcvol	146.510	ml/mol	McGowan Method
pc	3022.28	kPa	Joback Method
rinpol	1487.70		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	255.91		NIST Webbook
rinpol	254.57		NIST Webbook
rinpol	254.70		NIST Webbook

rinpol	1483.50		NIST Webbook
rinpol	256.69		NIST Webbook
rinpol	254.81		NIST Webbook
rinpol	263.90		NIST Webbook
rinpol	254.00		NIST Webbook
rinpol	263.90		NIST Webbook
rinpol	255.91		NIST Webbook
rinpol	254.81		NIST Webbook
rinpol	1474.50		NIST Webbook
rinpol	1487.70		NIST Webbook
rinpol	1464.00		NIST Webbook
rinpol	1487.70		NIST Webbook
rinpol	1475.60		NIST Webbook
rinpol	1483.50		NIST Webbook
rinpol	1464.40		NIST Webbook
rinpol	1474.50		NIST Webbook
rinpol	1480.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	254.33		NIST Webbook
rinpol	1474.50		NIST Webbook
ripol	2120.00		NIST Webbook
ripol	2104.00		NIST Webbook
ripol	2102.00		NIST Webbook
ripol	2102.00		NIST Webbook
tb	543.00 ± 5.00	K	NIST Webbook
tb	541.00 ± 4.00	K	NIST Webbook
tb	541.00 ± 4.00	K	NIST Webbook
tb	545.85 ± 1.00	K	NIST Webbook
tb	543.00 ± 3.00	K	NIST Webbook
tb	546.00 ± 4.00	K	NIST Webbook
tb	544.00 ± 4.00	K	NIST Webbook
tb	545.90	K	NIST Webbook
tb	548.00 ± 5.00	K	NIST Webbook
tc	800.99	K	Joback Method
tf	277.68 ± 0.10	K	NIST Webbook
tf	296.00 ± 2.00	K	NIST Webbook
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	407.46	J/mol×K	800.99	Joback Method
cpg	396.32	J/mol×K	760.03	Joback Method
cpg	384.20	J/mol×K	719.06	Joback Method
cpg	371.02	J/mol×K	678.09	Joback Method
cpg	356.73	J/mol×K	637.12	Joback Method
cpg	341.24	J/mol×K	596.15	Joback Method
cpg	324.50	J/mol×K	555.18	Joback Method
dvisc	0.0019527	Pa×s	301.63	Joback Method
dvisc	0.0001868	Pa×s	555.18	Joback Method
dvisc	0.0002351	Pa×s	512.92	Joback Method
dvisc	0.0003084	Pa×s	470.66	Joback Method
dvisc	0.0004268	Pa×s	428.40	Joback Method
dvisc	0.0006341	Pa×s	386.15	Joback Method
dvisc	0.0010384	Pa×s	343.89	Joback Method
hvapt	68.45	kJ/mol	298.15	Vapour pressures and enthalpies of vaporization of a series of the alkylbiphenyls

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45143e+01
Coeff. B	-4.46411e+03
Coeff. C	-9.28960e+01
Temperature range (K), min.	406.68
Temperature range (K), max.	577.98

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressures and enthalpies of vaporization of a series of the alkylbiphenyls:	https://www.doi.org/10.1016/j.fluid.2012.08.020
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=C643936&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume