

1,1'-Biphenyl, 2-ethyl-

Other names:	1-Ethyl-2-phenylbenzene 2-Ethylbiphenyl Biphenyl, 2-ethyl- o-Ethylbiphenyl
Inchi:	InChI=1S/C14H14/c1-2-12-8-6-7-11-14(12)13-9-4-3-5-10-13/h3-11H,2H2,1H3
InchiKey:	DLMYHUARHITGIJ-UHFFFAOYSA-N
Formula:	C14H14
SMILES:	CCc1ccccc1-c1ccccc1
Mol. weight [g/mol]:	182.26
CAS:	1812-51-7

Physical Properties

Property code	Value	Unit	Source
chl	-7280.00	kJ/mol	NIST Webbook
chl	-7585.20	kJ/mol	NIST Webbook
gf	282.19	kJ/mol	Joback Method
hf	129.30	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	51.97	kJ/mol	Joback Method
ie	8.55 ± 0.02	eV	NIST Webbook
log10ws	-4.88		Crippen Method
logp	3.916		Crippen Method
mcvol	160.600	ml/mol	McGowan Method
pc	2726.86	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	250.85		NIST Webbook
ripol	1994.00		NIST Webbook
ripol	2033.00		NIST Webbook
sl	332.69	J/mol×K	NIST Webbook
tb	539.12 ± 0.15	K	NIST Webbook
tb	539.12 ± 0.20	K	NIST Webbook
tc	818.72	K	Joback Method
tf	267.02 ± 0.10	K	NIST Webbook
tf	279.00 ± 2.00	K	NIST Webbook
tf	267.02 ± 0.10	K	NIST Webbook
tt	267.07 ± 0.01	K	NIST Webbook

vc

0.604

m³/kmol

Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.14	J/mol×K	578.06	Joback Method
cpg	389.56	J/mol×K	618.17	Joback Method
cpg	405.71	J/mol×K	658.28	Joback Method
cpg	420.65	J/mol×K	698.39	Joback Method
cpg	434.45	J/mol×K	738.50	Joback Method
cpg	447.19	J/mol×K	778.61	Joback Method
cpg	458.94	J/mol×K	818.72	Joback Method
cpl	302.73	J/mol×K	298.15	NIST Webbook
dvisc	0.0010159	Paxs	357.09	Joback Method
dvisc	0.0019467	Paxs	312.90	Joback Method
dvisc	0.0006118	Paxs	401.29	Joback Method
dvisc	0.0004075	Paxs	445.48	Joback Method
dvisc	0.0002920	Paxs	489.67	Joback Method
dvisc	0.0002212	Paxs	533.87	Joback Method
dvisc	0.0001748	Paxs	578.06	Joback Method
hfust	2.07	kJ/mol	267.08	NIST Webbook
hfust	2.07	kJ/mol	267.10	NIST Webbook
hfust	2.07	kJ/mol	267.10	NIST Webbook
sfust	7.74	J/mol×K	267.08	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	401.70	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$

Coeff. A	1.43677e+01
Coeff. B	-4.36865e+03
Coeff. C	-9.10250e+01
Temperature range (K), min.	401.30
Temperature range (K), max.	573.42

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1812517&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hfust:	Enthalpy of fusion at a given temperature
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
pvap:	Vapor pressure
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

tc: Critical Temperature
tf: Normal melting (fusion) point
tt: Triple Point Temperature
vc: Critical Volume

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