cis-Stilbene

Other names:	(1,2-Ethenediyl)-1,1'-bisbenzene, (Z)-
	(Z)-1,2-DIPHENYLETHYLENE
	(Z)-1,2-Diphenylethene
	(Z)-STILBENE
	1,1'-(1,2-Ethanediyl)bis[benzene], cis
	1,2-Diphenylethene, (Z)-
	1,cis-2-Diphenylethene
	1,cis-2-Diphenylethylene
	Benzene, 1,1'-(1,2-ethenediyl)bis-, (Z)-
	Benzene, 1,1'-(1,2-ethenedyl)bis-, (Z)-
	Benzene, 1,1'-(1Z)-1,2-ethenediylbis-
	CIS-1,2-DIPHENYLETHENE
	Dibenzal (cis)
	Isostilbene
	Stilbene, (Z)-
	cis-1,2-Diphenylethylene
	cis-Diphenylethene
Inchi:	InChI=1S/C14H12/c1-3-7-13(8-4-1)11-12-14-9-5-2-6-10-14/h1-12H/b12-11-
InchiKey:	PJANXHGTPQOBST-QXMHVHEDSA-N
Formula:	C14H12
SMILES:	C(=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	180.25
CAS:	645-49-8

Physical Properties

Property code	Value	Unit	Source
chl	-7407.60 ± 1.50	kJ/mol	NIST Webbook
chl	-7404.05 ± 0.75	kJ/mol	NIST Webbook
gf	372.04	kJ/mol	Joback Method
hf	257.99	kJ/mol	Joback Method
hfus	20.30	kJ/mol	Joback Method
hvap	50.30 ± 1.00	kJ/mol	NIST Webbook
hvap	70.50 ± 0.40	kJ/mol	NIST Webbook
hvap	66.00 ± 1.00	kJ/mol	NIST Webbook
ie	7.80 ± 0.02	eV	NIST Webbook
ie	8.17	eV	NIST Webbook
log10ws	-4.08		Crippen Method

logp	3.857		Crippen Method
mcvol	156.300	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1570.00		NIST Webbook
ripol	2205.00		NIST Webbook
tb	577.24	K	Joback Method
tc	828.15	K	Joback Method
tf	295.30	K	Joback Method
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.51	J/mol×K	828.15	Joback Method
cpg	352.81	J/mol×K	577.24	Joback Method
cpg	370.00	J/mol×K	619.06	Joback Method
cpg	385.74	J/mol×K	660.88	Joback Method
cpg	400.15	J/mol×K	702.70	Joback Method
cpg	413.35	J/mol×K	744.52	Joback Method
cpg	425.43	J/mol×K	786.33	Joback Method
dvisc	0.0001520	Pa×s	577.24	Joback Method
dvisc	0.0024141	Pa×s	295.30	Joback Method
dvisc	0.0011098	Pa×s	342.29	Joback Method
dvisc	0.0006154	Pa×s	389.28	Joback Method
dvisc	0.0003875	Pa×s	436.27	Joback Method
dvisc	0.0002670	Pa×s	483.26	Joback Method
dvisc	0.0001965	Pa×s	530.25	Joback Method
hsubt	90.80 ± 0.80	kJ/mol	329.00	NIST Webbook
hvapt	66.50	kJ/mol	400.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	356.20	K	0.05	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59981e+01
Coeff. B	-5.22261e+03
Coeff. C	-1.02293e+02
Temperature range (K), min.	434.72
Temperature range (K), max.	591.00

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.75110e+00
Coeff. B	-7.68079e+03
Coeff. C	1.63716e+00
Coeff. D	-3.53538e-06
Temperature range (K), min.	268.15
Temperature range (K), max.	535.00

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C645498&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=790

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

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

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

KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=790

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

Legend

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
hsubt:	Enthalpy of sublimation at a given temperature
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