(E)-Stilbene

Other names:	(1,2-Ethenediyl)-1,1'-bisbenzene, (E)-
	(E)-1,2-DIPHENYLETHYLENE
	(E)-1,2-Diphenylethene
	1,1'-(1,2-Ethanediyl)bis(benzene), (E)-
	1,1'-(1,2-Ethanediyl)bis[benzene], trans
	1,2-Diphenylethene, (E)-
	1,2-Diphenylethylene (trans)
	1,trans-2-Diphenylethene
	1,trans-2-Diphenylethylene
	Benzene, 1,1'-(1,2-ethenediyl)bis-, (E)-
	Benzene, 1,1'-(1E)-1,2-ethenediylbis-
	Dibenzal, (E)-
	Dibenzylidne, (E)-
	NSC 2069
	Stilbene (trans)
	Stilbene, (E)-
	TRANS-1,2-DIPHENYLETHTNE
	TRANS-STILBENE
	Toluylene
	t-Stilbene
	trans-1,2-Diphenylethene
	trans-1,2-Diphenylethylene
	trans-Bibenzal
	trans-Bibenzylidene
	trans-Diphenylethene
	trans-«alpha»,«beta»-Diphenylethylene
	trans-Â«alphaÂ»,Â«betaÂ»-Diphenylethylene
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-VAWYXSNFSA-N
Formula:	C14H12
SMILES:	C(=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	180.25
CAS:	103-30-0

Physical Properties

Property code	Value	Unit	Source

chl	-7360.99 ± 0.50	kJ/mol	NIST Webbook
chs	-7361.90 ± 2.80	kJ/mol	NIST Webbook
chs	-7364.60 ± 1.00	kJ/mol	NIST Webbook
chs	-7360.80 ± 3.90	kJ/mol	NIST Webbook
chs	-7357.10 ± 0.80	kJ/mol	NIST Webbook
ea	0.39 ± 0.02	eV	NIST Webbook
ea	0.39 ± 0.06	eV	NIST Webbook
gf	372.04	kJ/mol	Joback Method
hf	219.60	kJ/mol	NIST Webbook
hf	224.40	kJ/mol	NIST Webbook
hf	223.30	kJ/mol	NIST Webbook
hfs	137.80 ± 2.80	kJ/mol	NIST Webbook
hfs	136.70	kJ/mol	NIST Webbook
hfs	133.00 ± 0.80	kJ/mol	NIST Webbook
hfus	20.30	kJ/mol	Joback Method
hsub	102.00	kJ/mol	NIST Webbook
hsub	99.20 ± 0.40	kJ/mol	NIST Webbook
hsub	99.60 ± 1.70	kJ/mol	NIST Webbook
hsub	102.00 ± 0.40	kJ/mol	NIST Webbook
hsub	100.70 ± 0.40	kJ/mol	NIST Webbook
hsub	86.60	kJ/mol	NIST Webbook
hvap	79.70	kJ/mol	NIST Webbook
hvap	79.80	kJ/mol	NIST Webbook
hvap	79.60	kJ/mol	NIST Webbook
ie	7.66 ± 0.00	eV	NIST Webbook
ie	7.66 ± 0.00	eV	NIST Webbook
ie	7.87	eV	NIST Webbook
ie	7.91 ± 0.05	eV	NIST Webbook
ie	7.70 ± 0.02	eV	NIST Webbook
ie	7.76	eV	NIST Webbook
ie	7.70 ± 0.03	eV	NIST Webbook
ie	7.90 ± 0.05	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	1755.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1686.00		NIST Webbook
rinpol	1755.00		NIST Webbook
rinpol	1755.00		NIST Webbook
ripol	2536.00		NIST Webbook
ripol	2547.00		NIST Webbook
ripol	2536.00		NIST Webbook

ripol	2547.00		NIST Webbook
ss	247.00	J/mol×K	NIST Webbook
tb	579.55 ± 0.50	K	NIST Webbook
tc	828.15	K	Joback Method
tf	395.15 ± 2.00	K	NIST Webbook
tf	397.35	K	KDB
tf	397.00 ± 1.00	K	NIST Webbook
tf	397.60 ± 0.40	K	NIST Webbook
tf	394.00 ± 2.00	K	NIST Webbook
tf	397.00 ± 1.50	K	NIST Webbook
tf	397.00 ± 2.00	K	NIST Webbook
tf	397.00 ± 1.00	K	NIST Webbook
tt	398.00 ± 0.50	K	NIST Webbook
tt	397.40 ± 0.02	K	NIST Webbook
vc	0.584	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.74	J/mol×K	660.88	Joback Method
cpg	352.81	J/mol×K	577.24	Joback Method
cpg	436.51	J/mol×K	828.15	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
cpg	370.00	J/mol×K	619.06	Joback Method
cps	235.00	J/mol×K	298.15	NIST Webbook
cps	251.08	J/mol×K	320.00	NIST Webbook
dvisc	0.0001965	Pa×s	530.25	Joback Method
dvisc	0.0002670	Pa×s	483.26	Joback Method
dvisc	0.0024141	Pa×s	295.30	Joback Method
dvisc	0.0011098	Pa×s	342.29	Joback Method
dvisc	0.0001520	Pa×s	577.24	Joback Method
dvisc	0.0003875	Pa×s	436.27	Joback Method
dvisc	0.0006154	Pa×s	389.28	Joback Method
hfust	27.70	kJ/mol	397.40	NIST Webbook
hfust	27.40	kJ/mol	398.20	NIST Webbook
hfust	27.37	kJ/mol	398.00	NIST Webbook
hfust	27.40	kJ/mol	398.20	NIST Webbook
hsubt	99.60	kJ/mol	320.50	NIST Webbook
hsubt	90.80 ± 0.80	kJ/mol	329.00	NIST Webbook

hsubt	86.50 ± 0.10	kJ/mol	309.00	NIST Webbook
hsubt	103.80 ± 2.50	kJ/mol	315.50	NIST Webbook
hvapt	65.50	kJ/mol	499.50	NIST Webbook
sfust	68.80	J/mol×K	398.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	579.20	K	99.20	NIST Webbook
tbrp	439.70	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44500e+01
Coeff. B	-4.67696e+03
Coeff. C	-1.03848e+02
Temperature range (K), min.	434.08
Temperature range (K), max.	615.63

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.19966e+01
Coeff. B	-1.21896e+04
Coeff. C	-1.05568e+01
Coeff. D	2.37022e-06
Temperature range (K), min.	397.35
Temperature range (K), max.	820.00

Sources

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=791
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C103300&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=791
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
sfust:	Entropy of fusion at a given temperature
ss:	Solid 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