

1,3-Butadiene, 1,4-diphenyl-, (E,E)-

Other names:	trans,trans-1,4-Diphenyl-1,3-butadiene (E,E)-(C6H5CH=CH)2 (E,E)-1,4-Diphenyl-1,3-butadiene trans,trans-1,4-Diphenylbutadiene Benzene, 1,1'-(1,3-butadiene-1,4-diyl)bis-, (E,E)- 1,3-Butadiene, 1,4-diphenyl-, trans,trans- 1,4-Diphenyl-trans-1,trans-3-butadiene 1,4-Diphenyl-1,3-butadiene, trans,trans- (E,E)-1,4-Diphenylbutadiene all-trans-Diphenylbutadiene [(1E,3E)-4-Phenyl-1,3-butadienyl]benzene (1E,4E)-1,4-Diphenyl-1,3-butadiene (E,E)-(c6H5Ch=ch2)2
Inchi:	InChI=1S/C16H14/c1-3-9-15(10-4-1)13-7-8-14-16-11-5-2-6-12-16/h1-14H/b13-7+,14-8+
InchiKey:	JFLKFZNIIQFQBS-FNCQTZNRSA-N
Formula:	C16H14
SMILES:	C(C=Cc1ccccc1)=Cc1ccccc1
Mol. weight [g/mol]:	206.28
CAS:	538-81-8

Physical Properties

Property code	Value	Unit	Source
chs	-8475.70 ± 2.00	kJ/mol	NIST Webbook
chs	-8463.00 ± 6.70	kJ/mol	NIST Webbook
chs	-8493.10 ± 2.60	kJ/mol	NIST Webbook
gf	469.10	kJ/mol	Joback Method
hf	333.93	kJ/mol	Joback Method
hfus	25.68	kJ/mol	Joback Method
hvap	55.68	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.413		Crippen Method
mcvol	180.180	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
tb	623.20	K	NIST Webbook
tc	878.11	K	Joback Method
tf	426.40 ± 2.00	K	NIST Webbook
tf	425.90 ± 4.00	K	NIST Webbook

tf	423.70 ± 2.00	K	NIST Webbook
tf	421.40 ± 0.70	K	NIST Webbook
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.67	J/mol×K	627.16	Joback Method
cpg	448.24	J/mol×K	668.99	Joback Method
cpg	464.34	J/mol×K	710.81	Joback Method
cpg	479.08	J/mol×K	752.64	Joback Method
cpg	492.63	J/mol×K	794.46	Joback Method
cpg	505.13	J/mol×K	836.29	Joback Method
cpg	516.71	J/mol×K	878.11	Joback Method
dvisc	0.0021009	Pa×s	312.76	Joback Method
dvisc	0.0009047	Pa×s	365.16	Joback Method
dvisc	0.0004813	Pa×s	417.56	Joback Method
dvisc	0.0002948	Pa×s	469.96	Joback Method
dvisc	0.0001992	Pa×s	522.36	Joback Method
dvisc	0.0001446	Pa×s	574.76	Joback Method
dvisc	0.0001107	Pa×s	627.16	Joback Method
hsubt	166.00 ± 6.70	kJ/mol	293.00	NIST Webbook

Sources

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=C538818&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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