1,4-Diphenyl-1,3-butadiene

Other names: Benzene, 1,1'-(1,3-butadiene-1,4-diyl)bis-
1,3-Butadiene, 1,4-diphenyl-
Bistyryl
Distyryl
1,4-Diphenylbutadiene
1,4-Diphenylerythrene
(4-Phenyl-1,3-butadienyl)benzene
NSC 122702
1,4-diphenylbuta-1,3-diene

Inchi: InChI=1S/C16H14/c1-3-9-15(10-4-1)13-7-8-14-16-11-5-2-6-12-16/h1-14H

InchiKey: JFLKFZNIIQFQBS-UHFFFAOYSA-N

Formula: C16H14

SMILES: C(C=Cc1ccccc1)=Cc1ccccc1

Mol. weight [g/mol]: 206.28

CAS: 886-65-7

Physical Properties

Property code	Value	Unit	Source
ea	0.67 ± 0.02	eV	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
ie	7.56	eV	NIST Webbook
ie	7.75	eV	NIST Webbook
ie	7.54 ± 0.03	eV	NIST Webbook
ie	8.05	eV	NIST Webbook
log10ws	-4.77		Crippen Method
logp	4.413		Crippen Method
mcvol	180.180	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	1738.00		NIST Webbook
rinpol	1738.00		NIST Webbook
tb	627.16	K	Joback Method
tc	878.11	K	Joback Method
tf	425.00 ± 5.00	K	NIST Webbook
tf	425.90 ± 3.00	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

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=C886657&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume