

Benzene, 1,1'-(1,3,5-hexatriene-1,6-diyl)bis-

Other names:	1,3,5-Hexatriene, 1,6-diphenyl- Diphenylhexatriene 1,6-Diphenyl-1,3,5-hexatriene 1,6-Diphenylhexatriene a,w-Diphenylhexatriene Dph Dph (dye) Dicinnamyl (6-Phenyl-1,3,5-hexatrienyl)benzene 1,6-diphenylhexa-1,3,5-triene
Inchi:	InChI=1S/C18H16/c1(5-11-17-13-7-3-8-14-17)2-6-12-18-15-9-4-10-16-18/h1-16H/b2-1+,
InchiKey:	BOBLSBAZCVBABY-WPWUJOAOSA-N
Formula:	C18H16
SMILES:	C(=CC=Cc1ccccc1)C=Cc1ccccc1
Mol. weight [g/mol]:	232.32
CAS:	1720-32-7

Physical Properties

Property code	Value	Unit	Source
ea	0.89 ± 0.02	eV	NIST Webbook
gf	566.16	kJ/mol	Joback Method
hf	409.87	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	60.09	kJ/mol	Joback Method
ie	7.60	eV	NIST Webbook
ie	7.27 ± 0.03	eV	NIST Webbook
ie	7.33	eV	NIST Webbook
log10ws	-5.46		Crippen Method
logp	4.969		Crippen Method
mcvol	204.060	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
tb	677.08	K	Joback Method
tc	927.41	K	Joback Method
tf	475.20 ± 4.00	K	NIST Webbook
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	511.46	J/mol×K	677.08	Joback Method
cpg	529.13	J/mol×K	718.80	Joback Method
cpg	545.36	J/mol×K	760.52	Joback Method
cpg	560.31	J/mol×K	802.25	Joback Method
cpg	574.17	J/mol×K	843.97	Joback Method
cpg	587.10	J/mol×K	885.69	Joback Method
cpg	599.27	J/mol×K	927.41	Joback Method
dvisc	0.0017597	Pa×s	330.22	Joback Method
dvisc	0.0007135	Pa×s	388.03	Joback Method
dvisc	0.0003656	Pa×s	445.84	Joback Method
dvisc	0.0002184	Pa×s	503.65	Joback Method
dvisc	0.0001451	Pa×s	561.46	Joback Method
dvisc	0.0001040	Pa×s	619.27	Joback Method
dvisc	0.0000789	Pa×s	677.08	Joback Method

Sources

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=C1720327&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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