2,5-Diphenyl-2,4-hexadiene

Other names: [1-Methyl-4-phenyl-1,3-pentadienyl]benzene
2,4-Hexadiene, 2,5-diphenyl-
1,6-Diphenylhexadiene
Inchi: InChI=1S/C18H18/c1-15(17-9-5-3-6-10-17)13-14-16(2)18-11-7-4-8-12-18/h3-14H,1-2H3/
InchiKey: GGZMJMQKUXVBCQ-VMNXYWKNSA-N
Formula: C18H18
SMILES: CC(=CC=C(C)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 234.34
CAS: 16819-47-9

Physical Properties

Property code	Value	Unit	Source
gf	468.84	kJ/mol	Joback Method
hf	273.07	kJ/mol	Joback Method
hfus	28.24	kJ/mol	Joback Method
hvap	60.29	kJ/mol	Joback Method
ie	8.20	eV	NIST Webbook
log10ws	-5.60		Crippen Method
logp	5.193		Crippen Method
mcvol	208.360	ml/mol	McGowan Method
pc	2123.64	kPa	Joback Method
tb	672.68	K	Joback Method
tc	921.38	K	Joback Method
tf	307.38	K	Joback Method
vc	0.789	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.25	J/mol×K	672.68	Joback Method
cpg	552.07	J/mol×K	714.13	Joback Method
cpg	569.39	J/mol×K	755.58	Joback Method
cpg	585.37	J/mol×K	797.03	Joback Method
cpg	600.16	J/mol×K	838.48	Joback Method

cpg	613.90	J/mol×K	879.93	Joback Method
cpg	626.75	J/mol×K	921.38	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=C16819479&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
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