2,5-Diphenyl-1,5-hexadiene

Inchi: InChI=1S/C18H18/c1-15(17-9-5-3-6-10-17)13-14-16(2)18-11-7-4-8-12-18/h3-12H,1-2,13-
InchiKey: AJOYEXYQPJJGHQ-UHFFFAOYSA-N
Formula: C18H18
SMILES: C=C(CCC(=C)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 234.34
CAS: 7283-49-0

Physical Properties

Property code	Value	Unit	Source
gf	484.08	kJ/mol	Joback Method
hf	285.00	kJ/mol	NIST Webbook
hfus	25.28	kJ/mol	Joback Method
hvap	59.03	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.193		Crippen Method
mcvol	208.360	ml/mol	McGowan Method
pc	2085.03	kPa	Joback Method
tb	657.72	K	Joback Method
tc	896.31	K	Joback Method
tf	314.02	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.42	J/mol×K	657.72	Joback Method
cpg	550.15	J/mol×K	697.49	Joback Method
cpg	567.44	J/mol×K	737.25	Joback Method
cpg	583.40	J/mol×K	777.02	Joback Method
cpg	598.13	J/mol×K	816.78	Joback Method
cpg	611.75	J/mol×K	856.55	Joback Method
cpg	624.37	J/mol×K	896.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7283490&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
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