

1,4-Hexadiene, 2,5-diphenyl

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

Physical Properties

Property code	Value	Unit	Source
gf	476.46	kJ/mol	Joback Method
hf	281.28	kJ/mol	Joback Method
hfus	26.76	kJ/mol	Joback Method
hvap	59.66	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.193		Crippen Method
mcvol	208.360	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	1822.00		NIST Webbook
rinpol	1822.00		NIST Webbook
tb	665.20	K	Joback Method
tc	908.80	K	Joback Method
tf	310.70	K	Joback Method
vc	0.790	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.37	J/mol×K	665.20	Joback Method
cpg	551.15	J/mol×K	705.80	Joback Method
cpg	568.45	J/mol×K	746.40	Joback Method
cpg	584.41	J/mol×K	787.00	Joback Method
cpg	599.16	J/mol×K	827.60	Joback Method
cpg	612.83	J/mol×K	868.20	Joback Method
cpg	625.54	J/mol×K	908.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R72913&Units=SI

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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