

2,6-diphenyl-1,4-hexadiene

Inchi:	InChI=1S/C18H18/c1-16(18-14-6-3-7-15-18)10-8-9-13-17-11-4-2-5-12-17/h2-9,11-12,14-
InchiKey:	KMTSCEPZNOKULZ-HJWRWDBZSA-N
Formula:	C18H18
SMILES:	C=C(CC=CCc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	234.34

Physical Properties

Property code	Value	Unit	Source
gf	485.01	kJ/mol	Joback Method
hf	291.07	kJ/mol	Joback Method
hfus	28.07	kJ/mol	Joback Method
hvap	59.58	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.889		Crippen Method
mvol	208.360	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1927.70		NIST Webbook
rinpol	1927.70		NIST Webbook
tb	665.32	K	Joback Method
tc	904.69	K	Joback Method
tf	324.66	K	Joback Method
vc	0.789	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	532.66	J/mol×K	665.32	Joback Method
cpg	551.15	J/mol×K	705.22	Joback Method
cpg	568.21	J/mol×K	745.11	Joback Method
cpg	583.96	J/mol×K	785.01	Joback Method
cpg	598.53	J/mol×K	824.90	Joback Method
cpg	612.04	J/mol×K	864.80	Joback Method
cpg	624.60	J/mol×K	904.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R316331&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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