

2,6-diphenyl-2-hexene

Inchi:	InChI=1S/C18H20/c1-16(18-14-6-3-7-15-18)10-8-9-13-17-11-4-2-5-12-17/h2-7,10-12,14-
InchiKey:	KVNHMICZJAILQV-MHWRWJLKSA-N
Formula:	C18H20
SMILES:	CC(=CCCCc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	236.35

Physical Properties

Property code	Value	Unit	Source
gf	397.17	kJ/mol	Joback Method
hf	165.64	kJ/mol	Joback Method
hfus	29.35	kJ/mol	Joback Method
hvap	60.25	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	5.113		Crippen Method
mcvol	212.660	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	1914.30		NIST Webbook
tb	668.64	K	Joback Method
tc	903.14	K	Joback Method
tf	326.42	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.67	J/molxK	668.64	Joback Method
cpg	574.72	J/molxK	707.72	Joback Method
cpg	592.37	J/molxK	746.81	Joback Method
cpg	608.72	J/molxK	785.89	Joback Method
cpg	623.88	J/molxK	824.97	Joback Method
cpg	637.96	J/molxK	864.05	Joback Method
cpg	651.06	J/molxK	903.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R316346&Units=SI
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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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