

2,5-diphenyl-1,3-pentadiene

Inchi:	InChI=1S/C17H16/c1-15(17-13-6-3-7-14-17)9-8-12-16-10-4-2-5-11-16/h2-11,13-14H,1,12
InchiKey:	LOUCPTJGQXEIQI-CMDGGGOBGSA-N
Formula:	C17H16
SMILES:	<chem>C=C(C=CCc1ccccc1)c1ccccc1</chem>
Mol. weight [g/mol]:	220.31

Physical Properties

Property code	Value	Unit	Source
gf	476.59	kJ/mol	Joback Method
hf	311.71	kJ/mol	Joback Method
hfus	25.48	kJ/mol	Joback Method
hvap	57.36	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.499		Crippen Method
mvol	194.270	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1942.90		NIST Webbook
rinpol	1942.90		NIST Webbook
tb	642.44	K	Joback Method
tc	887.02	K	Joback Method
tf	313.39	K	Joback Method
vc	0.734	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.54	J/mol×K	642.44	Joback Method
cpg	498.74	J/mol×K	683.20	Joback Method
cpg	515.47	J/mol×K	723.97	Joback Method
cpg	530.86	J/mol×K	764.73	Joback Method
cpg	545.04	J/mol×K	805.49	Joback Method
cpg	558.14	J/mol×K	846.26	Joback Method
cpg	570.28	J/mol×K	887.02	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R316311&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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