

1,4-diphenyl-1,5-pentadiene

Inchi:	InChI=1S/C18H18/c1-2-9-17(18-12-7-4-8-13-18)15-14-16-10-5-3-6-11-16/h2-8,10-15,17H
InchiKey:	KBCQFLNZNSDIEU-CCEZHUSRSA-N
Formula:	C18H18
SMILES:	C=CCC(C=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]:	234.34

Physical Properties

Property code	Value	Unit	Source
gf	491.12	kJ/mol	Joback Method
hf	295.58	kJ/mol	Joback Method
hfus	25.86	kJ/mol	Joback Method
hvap	59.11	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	5.060		Crippen Method
mcvol	208.360	ml/mol	McGowan Method
pc	2100.34	kPa	Joback Method
rinpol	1786.40		NIST Webbook
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tb	665.00	K	Joback Method
tc	905.17	K	Joback Method
tf	323.62	K	Joback Method
vc	0.782	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.43	J/molxK	665.00	Joback Method
cpg	552.05	J/molxK	705.03	Joback Method
cpg	569.21	J/molxK	745.06	Joback Method
cpg	585.04	J/molxK	785.09	Joback Method
cpg	599.66	J/molxK	825.11	Joback Method
cpg	613.19	J/molxK	865.14	Joback Method
cpg	625.75	J/molxK	905.17	Joback Method
dvisc	0.0025465	Paxs	323.62	Joback Method

dvisc	0.0010009	Paxs	380.52	Joback Method
dvisc	0.0005016	Paxs	437.41	Joback Method
dvisc	0.0002947	Paxs	494.31	Joback Method
dvisc	0.0001932	Paxs	551.21	Joback Method
dvisc	0.0001371	Paxs	608.10	Joback Method
dvisc	0.0001032	Paxs	665.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R316222&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
dvisc:	Dynamic viscosity
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
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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