1,4-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/h2-14H,1H3/b12-8
InchiKey: KIHWPIBJULXNGT-VQDQISGBSA-N
Formula: C17H16
SMILES: CC(=CC=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 220.31

Physical Properties

Property code	Value	Unit	Source
gf	468.97	kJ/mol	Joback Method
hf	303.50	kJ/mol	Joback Method
hfus	26.96	kJ/mol	Joback Method
hvap	57.98	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.803		Crippen Method
mcvol	194.270	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinpol	1900.00		NIST Webbook
rinpol	1961.00		NIST Webbook
tb	649.92	K	Joback Method
tc	899.78	K	Joback Method
tf	310.07	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.33	J/mol×K	649.92	Joback Method
cpg	499.56	J/mol×K	691.56	Joback Method
cpg	516.31	J/mol×K	733.21	Joback Method
cpg	531.70	J/mol×K	774.85	Joback Method
cpg	545.90	J/mol×K	816.49	Joback Method
cpg	559.04	J/mol×K	858.14	Joback Method
cpg	571.27	J/mol×K	899.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R316044&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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