1,4-diphenyl-2-penten-2-one

Inchi: InChI=1S/C17H16O/c1-14(16-10-6-3-7-11-16)12-17(18)13-15-8-4-2-5-9-15/h2-12H,13H2
InchiKey: PKMNPZTZDALEFS-WYMLVPIESA-N
Formula: C17H16O
SMILES: CC(=CC(=O)Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 236.31

Physical Properties

Property code	Value	Unit	Source
gf	259.83	kJ/mol	Joback Method
hf	73.70	kJ/mol	Joback Method
hfus	28.36	kJ/mol	Joback Method
hvap	64.77	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.902		Crippen Method
mcvol	200.140	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
rinpol	2010.60		NIST Webbook
tb	699.63	K	Joback Method
tc	944.85	K	Joback Method
tf	365.08	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.72	J/mol×K	699.63	Joback Method
cpg	538.38	J/mol×K	740.50	Joback Method
cpg	553.69	J/mol×K	781.37	Joback Method
cpg	567.77	J/mol×K	822.24	Joback Method
cpg	580.73	J/mol×K	863.11	Joback Method
cpg	592.68	J/mol×K	903.98	Joback Method
cpg	603.75	J/mol×K	944.85	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R316237&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
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
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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