2,4-diphenyl-1-buten-4-one

Inchi: InChI=1S/C16H14O/c1-13(14-8-4-2-5-9-14)12-16(17)15-10-6-3-7-11-15/h2-11H,1,12H2
InchiKey: IARGMAYLOFUHTE-UHFFFAOYSA-N
Formula: C16H14O
SMILES: C=C(CC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
gf	259.03	kJ/mol	Joback Method
hf	102.55	kJ/mol	Joback Method
hfus	24.29	kJ/mol	Joback Method
hvap	61.92	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	3.973		Crippen Method
mcvol	186.050	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1887.20		NIST Webbook
rinpol	1887.20		NIST Webbook
tb	669.27	K	Joback Method
tc	914.88	K	Joback Method
tf	357.13	K	Joback Method
vc	0.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.22	J/mol×K	669.27	Joback Method
cpg	485.52	J/mol×K	710.20	Joback Method
cpg	500.47	J/mol×K	751.14	Joback Method
cpg	514.16	J/mol×K	792.07	Joback Method
cpg	526.70	J/mol×K	833.01	Joback Method
cpg	538.18	J/mol×K	873.94	Joback Method
cpg	548.71	J/mol×K	914.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R316079&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