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

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

Physical Properties

Property code	Value	Unit	Source
gf	267.45	kJ/mol	Joback Method
hf	81.91	kJ/mol	Joback Method
hfus	26.88	kJ/mol	Joback Method
hvap	64.14	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	4.363		Crippen Method
mcvol	200.140	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpol	2175.00		NIST Webbook
rinpol	2175.00		NIST Webbook
tb	692.15	K	Joback Method
tc	932.54	K	Joback Method
tf	368.40	K	Joback Method
vc	0.759	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.24	J/mol×K	692.15	Joback Method
cpg	537.88	J/mol×K	732.21	Joback Method
cpg	553.18	J/mol×K	772.28	Joback Method
cpg	567.25	J/mol×K	812.34	Joback Method
cpg	580.18	J/mol×K	852.41	Joback Method
cpg	592.07	J/mol×K	892.47	Joback Method
cpg	603.01	J/mol×K	932.54	Joback Method

Sources

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=R316257&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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