1,4-Diphenyl-1-pentanone

Inchi: InChI=1S/C17H18O/c1-14(15-8-4-2-5-9-15)12-13-17(18)16-10-6-3-7-11-16/h2-11,14H,12
InchiKey: NWTNYXHABGPXMO-UHFFFAOYSA-N
Formula: C17H18O
SMILES: CC(CCC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 238.32
CAS: 72256-08-7

Physical Properties

Property code	Value	Unit	Source
gf	185.72	kJ/mol	Joback Method
hf	-39.01	kJ/mol	Joback Method
hfus	25.94	kJ/mol	Joback Method
hvap	64.35	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.453		Crippen Method
mcvol	204.440	ml/mol	McGowan Method
pc	2231.30	kPa	Joback Method
rinpol	2164.30		NIST Webbook
rinpol	2164.30		NIST Webbook
tb	695.15	K	Joback Method
tc	931.51	K	Joback Method
tf	369.12	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.63	J/mol×K	695.15	Joback Method
cpg	619.70	J/mol×K	892.12	Joback Method
cpg	607.25	J/mol×K	852.72	Joback Method
cpg	593.70	J/mol×K	813.33	Joback Method
cpg	578.97	J/mol×K	773.94	Joback Method
cpg	562.98	J/mol×K	734.54	Joback Method
cpg	631.14	J/mol×K	931.51	Joback Method

dvisc	0.0001297	Pa×s	695.15	Joback Method
dvisc	0.0001709	Pa×s	640.81	Joback Method
dvisc	0.0002370	Pa×s	586.47	Joback Method
dvisc	0.0003514	Pa×s	532.13	Joback Method
dvisc	0.0005699	Pa×s	477.80	Joback Method
dvisc	0.0010462	Pa×s	423.46	Joback Method
dvisc	0.0022968	Pa×s	369.12	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=C72256087&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
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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