1,4-diphenyl-3-buten-2-one

Inchi: InChI=1S/C16H14O/c17-16(13-15-9-5-2-6-10-15)12-11-14-7-3-1-4-8-14/h1-12H,13H2/b1
InchiKey: QMDWBHJPUAOGHO-VAWYXSNFSA-N
Formula: C16H14O
SMILES: O=C(C=Cc1ccccc1)Cc1ccccc1
Mol. weight [g/mol]: 222.28

Physical Properties

Property code	Value	Unit	Source
gf	259.96	kJ/mol	Joback Method
hf	104.13	kJ/mol	Joback Method
hfus	27.08	kJ/mol	Joback Method
hvap	62.47	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.512		Crippen Method
mcvol	186.050	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	2038.90		NIST Webbook
tb	676.87	K	Joback Method
tc	923.21	K	Joback Method
tf	367.77	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.90	J/mol×K	676.87	Joback Method
cpg	485.96	J/mol×K	717.93	Joback Method
cpg	500.69	J/mol×K	758.98	Joback Method
cpg	514.20	J/mol×K	800.04	Joback Method
cpg	526.60	J/mol×K	841.10	Joback Method
cpg	538.00	J/mol×K	882.15	Joback Method
cpg	548.51	J/mol×K	923.21	Joback Method
dvisc	0.0018365	Pa×s	367.77	Joback Method
dvisc	0.0009086	Pa×s	419.29	Joback Method

dvisc	0.0005244	Pa×s	470.80	Joback Method
dvisc	0.0003373	Pa×s	522.32	Joback Method
dvisc	0.0002349	Pa×s	573.84	Joback Method
dvisc	0.0001736	Pa×s	625.35	Joback Method
dvisc	0.0001343	Pa×s	676.87	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R316242&Units=SI

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