1-Butanone, 1,4-diphenyl-

Other names: 4-Phenylbutyrophenone
1,4-Diphenyl-1-butanone
Inchi: InChI=1S/C16H16O/c17-16(15-11-5-2-6-12-15)13-7-10-14-8-3-1-4-9-14/h1-6,8-9,11-12H
InchiKey: GBUMEGLMTNAXOM-UHFFFAOYSA-N
Formula: C16H16O
SMILES: O=C(CCCc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 224.30
CAS: 5407-91-0

Physical Properties

Property code	Value	Unit	Source
gf	179.74	kJ/mol	Joback Method
hf	-13.09	kJ/mol	Joback Method
hfus	26.88	kJ/mol	Joback Method
hvap	62.51	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.892		Crippen Method
mcvol	190.350	ml/mol	McGowan Method
pc	2429.05	kPa	Joback Method
rinpol	1851.20		NIST Webbook
tb	672.71	K	Joback Method
tc	909.11	K	Joback Method
tf	372.85	K	Joback Method
vc	0.722	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.41	J/mol×K	672.71	Joback Method
cpg	509.09	J/mol×K	712.11	Joback Method
cpg	524.47	J/mol×K	751.51	Joback Method
cpg	538.63	J/mol×K	790.91	Joback Method
cpg	551.66	J/mol×K	830.31	Joback Method
cpg	563.63	J/mol×K	869.71	Joback Method

cpg	574.64	J/mol×K	909.11	Joback Method
dvisc	0.0019909	Pa×s	372.85	Joback Method
dvisc	0.0010134	Pa×s	422.83	Joback Method
dvisc	0.0005950	Pa×s	472.80	Joback Method
dvisc	0.0003868	Pa×s	522.78	Joback Method
dvisc	0.0002711	Pa×s	572.76	Joback Method
dvisc	0.0002011	Pa×s	622.73	Joback Method
dvisc	0.0001560	Pa×s	672.71	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5407910&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
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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