4-tert-Butyl-benzophenone

Other names:	4-(t-Butyl)benzophenone
	Methanone, [4-(1,1-dimethylethyl)phenyl]phenyl-
Inchi:	InChI=1S/C17H18O/c1-17(2,3)15-11-9-14(10-12-15)16(18)13-7-5-4-6-8-13/h4-12H,1-3H
InchiKey:	DFYJCXSOGSYMAJ-UHFFFAOYSA-N
Formula:	C17H18O
SMILES:	CC(C)(C)c1ccc(C(=O)c2ccccc2)cc1
Mol. weight [g/mol]:	238.32
CAS:	22679-54-5

Physical Properties

Property code	Value	Unit	Source
chl	-9127.00 ± 2.00	kJ/mol	NIST Webbook
gf	181.37	kJ/mol	Joback Method
hf	-53.95	kJ/mol	Joback Method
hfl	-136.00	kJ/mol	NIST Webbook
hfus	21.66	kJ/mol	Joback Method
hvap	64.10	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.215		Crippen Method
mcvol	204.440	ml/mol	McGowan Method
pc	2222.89	kPa	Joback Method
tb	697.34	K	Joback Method
tc	943.53	K	Joback Method
tf	399.06	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.01	J/mol×K	697.34	Joback Method
cpg	564.48	J/mol×K	738.37	Joback Method
cpg	580.50	J/mol×K	779.40	Joback Method
cpg	595.19	J/mol×K	820.43	Joback Method
cpg	608.67	J/mol×K	861.47	Joback Method

cpg	621.06	J/mol×K	902.50	Joback Method
cpg	632.46	J/mol×K	943.53	Joback Method
dvisc	0.0015610	Pa×s	399.06	Joback Method
dvisc	0.0007988	Pa×s	448.77	Joback Method
dvisc	0.0004672	Pa×s	498.49	Joback Method
dvisc	0.0003012	Pa×s	548.20	Joback Method
dvisc	0.0002089	Pa×s	597.91	Joback Method
dvisc	0.0001532	Pa×s	647.63	Joback Method
dvisc	0.0001175	Pa×s	697.34	Joback Method

Sources

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=C22679545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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