4'-tert-Butyl-2',6'-dimethylacetophenone

Other names:	4-t-Butyl-2,6-dimethylacetophenone
	4-tert-Butyl-2,6-dimethylacetophenone
	Ethanone, 1-[4-(1,1-dimethylethyl)-2,6-dimethylphenyl]-
	Acetophenone, 4'-tert-butyl-2',6'-dimethyl-
Inchi:	InChI=1S/C14H20O/c1-9-7-12(14(4,5)6)8-10(2)13(9)11(3)15/h7-8H,1-6H3
InchiKey:	JNHLHPMTMTYLCP-UHFFFAOYSA-N
Formula:	C14H20O
SMILES:	CC(=O)c1c(C)cc(C(C)(C)C)cc1C
Mol. weight [g/mol]:	204.31
CAS:	2040-10-0

Physical Properties

Property code	Value	Unit	Source
gf	24.44	kJ/mol	Joback Method
hf	-251.50	kJ/mol	Joback Method
hfus	19.07	kJ/mol	Joback Method
hvap	56.47	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.804		Crippen Method
mcvol	185.930	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
tb	611.98	K	Joback Method
tc	828.53	K	Joback Method
tf	363.87	K	Joback Method
vc	0.707	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.43	J/mol×K	611.98	Joback Method
cpg	486.29	J/mol×K	648.07	Joback Method
cpg	502.13	J/mol×K	684.16	Joback Method
cpg	517.00	J/mol×K	720.26	Joback Method
cpg	530.94	J/mol×K	756.35	Joback Method

cpg	544.00	J/mol×K	792.44	Joback Method
cpg	556.23	J/mol×K	828.53	Joback Method
dvisc	0.0014848	Pa×s	363.87	Joback Method
dvisc	0.0008485	Pa×s	405.22	Joback Method
dvisc	0.0005379	Pa×s	446.57	Joback Method
dvisc	0.0003683	Pa×s	487.93	Joback Method
dvisc	0.0002676	Pa×s	529.28	Joback Method
dvisc	0.0002036	Pa×s	570.63	Joback Method
dvisc	0.0001608	Pa×s	611.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2040100&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.