Phenyl tert-butyl ketone

Other names:	1-Propanone, 2,2-dimethyl-1-phenyl- Pivalophenone «alpha»,«alpha»-Dimethylpropiophenone tert-Butyl Phenyl ketone 2,2-Dimethylpropiophenone 2,2-Dimethyl-1-phenyl-1-propanone
Inchi:	InChI=1S/C11H14O/c1-11(2,3)10(12)9-7-5-4-6-8-9/h4-8H,1-3H3
InchiKey:	OECPUBRNDKXFDX-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	CC(C)(C)C(=O)c1ccccc1
Mol. weight [g/mol]:	162.23
CAS:	938-16-9

Physical Properties

Property code	Value	Unit	Source
chl	-6120.70 ± 2.30	kJ/mol	NIST Webbook
gf	28.07	kJ/mol	Joback Method
hf	-155.17	kJ/mol	Joback Method
hfl	-208.80 ± 2.50	kJ/mol	NIST Webbook
hfus	12.47	kJ/mol	Joback Method
hvap	47.81	kJ/mol	Joback Method
ie	8.98	eV	NIST Webbook
ie	9.02	eV	NIST Webbook
ie	9.04 ± 0.04	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
log10ws	-3.15		Crippen Method
logp	2.915		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2887.40	kPa	Joback Method
rinpol	1233.00		NIST Webbook
tb	493.20	K	NIST Webbook
tc	753.70	K	Joback Method
tf	292.50	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.62	J/mol×K	753.70	Joback Method
cpg	393.75	J/mol×K	716.15	Joback Method
cpg	382.00	J/mol×K	678.60	Joback Method
cpg	369.30	J/mol×K	641.05	Joback Method
cpg	355.60	J/mol×K	603.50	Joback Method
cpg	340.81	J/mol×K	565.95	Joback Method
cpg	324.88	J/mol×K	528.40	Joback Method
dvisc	0.0039648	Pa×s	292.50	Joback Method
dvisc	0.0002297	Pa×s	528.40	Joback Method
dvisc	0.0003051	Pa×s	489.08	Joback Method
dvisc	0.0004259	Pa×s	449.77	Joback Method
dvisc	0.0006337	Pa×s	410.45	Joback Method
dvisc	0.0010259	Pa×s	371.13	Joback Method
dvisc	0.0018616	Pa×s	331.82	Joback Method
hvapt	55.50	kJ/mol	411.50	NIST Webbook

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=C938169&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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