Ethanone, 1-[4-(1,1-dimethylethyl)phenyl]-

Other names:	Acetophenone, 4'-tert-butyl-
	p-tert-Butylacetophenone
	4-tert-Butylacetophenone
	4'-tert-Butylacetophenone
	4'-t-Butylacetophenone
	1-(4-Tert-butylphenyl)ethanone
Inchi:	InChI=1S/C12H16O/c1-9(13)10-5-7-11(8-6-10)12(2,3)4/h5-8H,1-4H3
InchiKey:	UYFJYGWNYQCHOB-UHFFFAOYSA-N
Formula:	C12H16O
SMILES:	CC(=O)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	176.25
CAS:	943-27-1

Physical Properties

Property code	Value	Unit	Source
affp	882.50	kJ/mol	NIST Webbook
basg	850.60	kJ/mol	NIST Webbook
gf	26.86	kJ/mol	Joback Method
hf	-187.28	kJ/mol	Joback Method
hfus	14.67	kJ/mol	Joback Method
hvap	50.69	kJ/mol	Joback Method
ie	9.01 ± 0.05	eV	NIST Webbook
log10ws	-3.45		Crippen Method
logp	3.187		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
tb	556.26	K	Joback Method
tc	778.63	K	Joback Method
tf	316.29	K	Joback Method
vc	0.595	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	371.63	J/mol×K	556.26	Joback Method
cpg	442.58	J/mol×K	741.57	Joback Method
cpg	430.34	J/mol×K	704.51	Joback Method
cpg	417.19	J/mol×K	667.45	Joback Method
cpg	403.06	J/mol×K	630.38	Joback Method
cpg	387.90	J/mol×K	593.32	Joback Method
cpg	453.96	J/mol×K	778.63	Joback Method
dvisc	0.0002033	Pa×s	556.26	Joback Method
dvisc	0.0002652	Pa×s	516.26	Joback Method
dvisc	0.0003618	Pa×s	476.27	Joback Method
dvisc	0.0005225	Pa×s	436.27	Joback Method
dvisc	0.0008127	Pa×s	396.28	Joback Method
dvisc	0.0013958	Pa×s	356.29	Joback Method
dvisc	0.0027486	Pa×s	316.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.70	K	0.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C943271&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

Legend

affp: Proton affinity
basg: Gas basicity
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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume