4'-Methylbutyrophenone

Other names:	4-Methylbutyrophenone
	p-Methyl butyrophenone
	1-Butanone, 1-(4-methylphenyl)-
	Butyrophenone, 4'-methyl-
	1-(4-Tolyl)-1-butanone
Inchi:	InChI=1S/C11H14O/c1-3-4-11(12)10-7-5-9(2)6-8-10/h5-8H,3-4H2,1-2H3
InchiKey:	CIYAESDXUTVTAL-UHFFFAOYSA-N
Formula:	C11H14O
SMILES:	CCCC(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	162.23
CAS:	4160-52-5

Physical Properties

Property code	Value	Unit	Source
gf	15.60	kJ/mol	Joback Method
hf	-157.89	kJ/mol	Joback Method
hfus	19.50	kJ/mol	Joback Method
hvap	49.76	kJ/mol	Joback Method
ie	8.80 ± 0.20	eV	NIST Webbook
log10ws	-3.44		Crippen Method
logp	2.978		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2784.72	kPa	Joback Method
tb	536.61	K	Joback Method
tc	749.19	K	Joback Method
tf	302.60	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.61	J/mol×K	536.61	Joback Method
cpg	336.08	J/mol×K	572.04	Joback Method
cpg	349.73	J/mol×K	607.47	Joback Method

cpg	362.58	J/mol×K	642.90	Joback Method
cpg	374.66	J/mol×K	678.33	Joback Method
cpg	386.00	J/mol×K	713.76	Joback Method
cpg	396.64	J/mol×K	749.19	Joback Method
dvisc	0.0022892	Pa×s	302.60	Joback Method
dvisc	0.0012638	Pa×s	341.60	Joback Method
dvisc	0.0007880	Pa×s	380.60	Joback Method
dvisc	0.0005365	Pa×s	419.60	Joback Method
dvisc	0.0003899	Pa×s	458.61	Joback Method
dvisc	0.0002979	Pa×s	497.61	Joback Method
dvisc	0.0002367	Pa×s	536.61	Joback Method

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=C4160525&Units=SI

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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume