1-Butanone, 1-(4-chlorophenyl)-

Other names: Butyrophenone, 4'-chloro-
p-Chlorobutyrophenone
4-Chlorophenyl propyl ketone
4'-Chlorobutyrophenone
1-(4-Chlorophenyl)-1-butanone
Inchi: InChI=1S/C10H11ClO/c1-2-3-10(12)8-4-6-9(11)7-5-8/h4-7H,2-3H2,1H3
InchiKey: XLCJPQYALLFIPW-UHFFFAOYSA-N
Formula: C10H11ClO
SMILES: CCCC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 182.65
CAS: 4981-63-9

Physical Properties

Property code	Value	Unit	Source
gf	-4.75	kJ/mol	Joback Method
hf	-152.99	kJ/mol	Joback Method
hfus	21.10	kJ/mol	Joback Method
hvap	51.92	kJ/mol	Joback Method
ie	9.00 ± 0.20	eV	NIST Webbook
log10ws	-3.65		Crippen Method
logp	3.323		Crippen Method
mcvol	141.810	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1586.00		NIST Webbook
rinpol	1586.00		NIST Webbook
tb	551.16	K	Joback Method
tc	771.98	K	Joback Method
tf	321.25	K	Joback Method
vc	0.542	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.67	J/mol×K	551.16	Joback Method

cpg	315.41	J/mol×K	587.96	Joback Method
cpg	327.34	J/mol×K	624.77	Joback Method
cpg	338.51	J/mol×K	661.57	Joback Method
cpg	348.95	J/mol×K	698.37	Joback Method
cpg	358.68	J/mol×K	735.18	Joback Method
cpg	367.75	J/mol×K	771.98	Joback Method
dvisc	0.0022030	Pa×s	321.25	Joback Method
dvisc	0.0012737	Pa×s	359.57	Joback Method
dvisc	0.0008183	Pa×s	397.89	Joback Method
dvisc	0.0005683	Pa×s	436.20	Joback Method
dvisc	0.0004186	Pa×s	474.52	Joback Method
dvisc	0.0003227	Pa×s	512.84	Joback Method
dvisc	0.0002580	Pa×s	551.16	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=C4981639&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume