p-(Chlorophenyl)acetone

Other names:	2-Propanone, 1-(4-chlorophenyl)- 2-Propanone,p-chlorophenyl- 1-(p-Chlorophenyl)acetone NSC 22985 Methyl p-chlorobenzyl ketone
Inchi:	InChI=1S/C9H9ClO/c1-7(11)6-8-2-4-9(10)5-3-8/h2-5H,6H2,1H3
InchiKey:	WEJRYKSUUFKMBC-UHFFFAOYSA-N
Formula:	C9H9ClO
SMILES:	CC(=O)Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	168.62
CAS:	5586-88-9

Physical Properties

Property code	Value	Unit	Source
gf	-13.17	kJ/mol	Joback Method
hf	-132.35	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	49.70	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.471		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
pc	3302.95	kPa	Joback Method
tb	528.28	K	Joback Method
tc	753.10	K	Joback Method
tf	309.98	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.49	J/mol×K	528.28	Joback Method
cpg	310.02	J/mol×K	715.63	Joback Method
cpg	301.10	J/mol×K	678.16	Joback Method
cpg	291.51	J/mol×K	640.69	Joback Method

cpg	281.24	J/mol×K	603.22	Joback Method
cpg	270.24	J/mol×K	565.75	Joback Method
cpg	318.31	J/mol×K	753.10	Joback Method
dvisc	0.0002769	Pa×s	528.28	Joback Method
dvisc	0.0003443	Pa×s	491.90	Joback Method
dvisc	0.0004434	Pa×s	455.51	Joback Method
dvisc	0.0005966	Pa×s	419.13	Joback Method
dvisc	0.0008494	Pa×s	382.75	Joback Method
dvisc	0.0013025	Pa×s	346.36	Joback Method
dvisc	0.0022080	Pa×s	309.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5586889&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

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