1-Propanone, 3-chloro-1-phenyl-

Other names:	«beta»-Chloropropiophenone
	«omega»-Chloropropiophenone
	«beta»-Chloroethyl phenyl ketone
	Propiophenone, 3-chloro-
	2-Chloroethyl phenyl ketone
	3-Chloropropanophenone
	3-Chloropropiophenone
	3-Chloro-1-phenyl-1-propanone
	NSC 227202
	NSC 37238
Inchi:	InChI=1S/C9H9ClO/c10-7-6-9(11)8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey:	KTJRGPZVSKWRTJ-UHFFFAOYSA-N
Formula:	C9H9ClO
SMILES:	O=C(CCCl)c1ccccc1
Mol. weight [g/mol]:	168.62
CAS:	936-59-4

Physical Properties

Property code	Value	Unit	Source
gf	-3.54	kJ/mol	Joback Method
hf	-120.88	kJ/mol	Joback Method
hfus	18.90	kJ/mol	Joback Method
hvap	49.03	kJ/mol	Joback Method
log10ws	-2.70		Crippen Method
logp	2.498		Crippen Method
mcvol	127.720	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	1378.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1390.00		NIST Webbook
tb	523.30	K	Joback Method
tc	746.94	K	Joback Method
tf	297.46	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.91	J/mol×K	523.30	Joback Method
cpg	271.02	J/mol×K	560.57	Joback Method
cpg	282.32	J/mol×K	597.85	Joback Method
cpg	292.84	J/mol×K	635.12	Joback Method
cpg	302.62	J/mol×K	672.39	Joback Method
cpg	311.69	J/mol×K	709.67	Joback Method
cpg	320.10	J/mol×K	746.94	Joback Method
dvisc	0.0029503	Pa×s	297.46	Joback Method
dvisc	0.0016071	Pa×s	335.10	Joback Method
dvisc	0.0009896	Pa×s	372.74	Joback Method
dvisc	0.0006661	Pa×s	410.38	Joback Method
dvisc	0.0004792	Pa×s	448.02	Joback Method
dvisc	0.0003628	Pa×s	485.66	Joback Method
dvisc	0.0002859	Pa×s	523.30	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.20	K	0.50	NIST Webbook

Sources

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=C936594&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume