

2-Pentanone, 5-chloro-

Other names:	1-chloro-4-pentanone 3-Acetylpropyl chloride 3-chloropropyl methyl ketone 5-chloro-2-pentanone 5-chloropentan-2-one
Inchi:	InChI=1S/C5H9ClO/c1-5(7)3-2-4-6/h2-4H2,1H3
InchiKey:	XVRIEWDDMODMGA-UHFFFAOYSA-N
Formula:	C5H9ClO
SMILES:	CC(=O)CCCCl
Mol. weight [g/mol]:	120.58
CAS:	5891-21-4

Physical Properties

Property code	Value	Unit	Source
gf	-149.63	kJ/mol	Joback Method
hf	-274.85	kJ/mol	Joback Method
hfus	14.50	kJ/mol	Joback Method
hvap	37.86	kJ/mol	Joback Method
log10ws	-1.35		Crippen Method
logp	1.594		Crippen Method
mvol	95.120	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	965.00		NIST Webbook
rinpol	965.00		NIST Webbook
tb	405.10	K	Joback Method
tc	591.48	K	Joback Method
tf	225.96	K	Joback Method
vc	0.370	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.83	J/molxK	591.48	Joback Method
cpg	174.65	J/molxK	436.16	Joback Method

cpg	182.77	J/molxK	467.23	Joback Method
cpg	190.54	J/molxK	498.29	Joback Method
cpg	197.97	J/molxK	529.35	Joback Method
cpg	205.06	J/molxK	560.42	Joback Method
cpg	166.17	J/molxK	405.10	Joback Method
dvisc	0.0037554	Paxs	225.96	Joback Method
dvisc	0.0020219	Paxs	255.82	Joback Method
dvisc	0.0012390	Paxs	285.67	Joback Method
dvisc	0.0008330	Paxs	315.53	Joback Method
dvisc	0.0005998	Paxs	345.39	Joback Method
dvisc	0.0004551	Paxs	375.24	Joback Method
dvisc	0.0003596	Paxs	405.10	Joback Method
pvap	103.42	kPa	454.00	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	92.85	kPa	449.30	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	81.58	kPa	443.60	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone

pvap	72.35	kPa	438.10	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	62.27	kPa	433.50	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	52.60	kPa	423.80	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	41.16	kPa	413.80	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone

pvap	30.23	kPa	404.60	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	20.79	kPa	393.80	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	10.50	kPa	373.80	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	7.15	kPa	363.10	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone

pvap	4.66	kPa	353.10	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone
pvap	2.91	kPa	343.20	Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	344.70	K	2.70	NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

Density, Viscosity, and Vapor-Liquid Equilibrium Data for the Binary Mixture at Atmosphere Pressure: Cyclopropyl Methyl Ketone + 2-Acetylbutyrolactone, Cyclopropyl Methyl Ketone + 5-Chloro-2-pentanone: <https://www.doi.org/10.1021/acs.jced.7b00344>

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=C5891214&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpolar:	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

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