1-Chloro-3-pentanone

Other names:	3-Pentanone, 1-chloro-
	«beta»-Chloroethyl ethyl ketone
	1-Chloroethyl ethyl ketone
	1-chloropentan-3-one
Inchi:	InChI=1S/C5H9ClO/c1-2-5(7)3-4-6/h2-4H2,1H3
InchiKey:	APNSUHRNUVUCIP-UHFFFAOYSA-N
Formula:	C5H9ClO
SMILES:	CCC(=O)CCCl
Mol. weight [g/mol]:	120.58
CAS:	32830-97-0

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
mcvol	95.120	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
tb	405.10	K	Joback Method
tc	591.48	K	Joback Method
tf	225.96	K	Joback Method
vc	0.370	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.17	J/mol×K	405.10	Joback Method
cpg	174.65	J/mol×K	436.16	Joback Method
cpg	182.77	J/mol×K	467.23	Joback Method
cpg	190.54	J/mol×K	498.29	Joback Method
cpg	197.97	J/mol×K	529.35	Joback Method

cpg	205.06	J/mol×K	560.42	Joback Method
cpg	211.83	J/mol×K	591.48	Joback Method
dvisc	0.0037554	Pa×s	225.96	Joback Method
dvisc	0.0020219	Pa×s	255.82	Joback Method
dvisc	0.0012390	Pa×s	285.67	Joback Method
dvisc	0.0008330	Pa×s	315.53	Joback Method
dvisc	0.0005998	Pa×s	345.39	Joback Method
dvisc	0.0004551	Pa×s	375.24	Joback Method
dvisc	0.0003596	Pa×s	405.10	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.20	K	2.70	NIST Webbook

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=C32830970&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume