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

Physical Properties

Property code	Value	Unit	Source
af	0.3858		Cheméo Relay (1.0)
gf	-149.63	kJ/mol	Joback Method
hf	-289.31	kJ/mol	Cheméo Relay (1.0)
hfus	14.50	kJ/mol	Joback Method
hvap	43.37	kJ/mol	Cheméo Relay (1.0)
ie	9.76	eV	Cheméo Relay (1.0)
log10ws	-0.78		Cheméo Relay (1.0)
logp	1.594		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
tb	433.13	K	Cheméo Relay (1.0)
tc	616.26	K	Cheméo Relay (1.0)
tf	273.51	K	Cheméo Relay (1.0)
vc	0.336	m3/kmol	Cheméo Relay (1.0)

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: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C32830970&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume