4-Chloro-2-butanone

Other names: 2-Butanone, 4-chloro-
1-Chloro-3-butanone
4-chlorobutan-2-one
Inchi: InChI=1S/C4H7ClO/c1-4(6)2-3-5/h2-3H2,1H3
InchiKey: MAGOYBJJLVSJIC-UHFFFAOYSA-N
Formula: C4H7ClO
SMILES: CC(=O)CCCl
Mol. weight [g/mol]: 106.55
CAS: 6322-49-2

Physical Properties

Property code	Value	Unit	Source
gf	-158.05	kJ/mol	Joback Method
hf	-254.21	kJ/mol	Joback Method
hfus	11.91	kJ/mol	Joback Method
hvap	35.63	kJ/mol	Joback Method
log10ws	-0.93		Crippen Method
logp	1.204		Crippen Method
mcvol	81.030	ml/mol	McGowan Method
pc	4026.13	kPa	Joback Method
rinpol	760.00		NIST Webbook
tb	382.22	K	Joback Method
tc	569.79	K	Joback Method
tf	214.69	K	Joback Method
vc	0.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	131.57	J/mol×K	382.22	Joback Method
cpg	138.59	J/mol×K	413.48	Joback Method
cpg	145.30	J/mol×K	444.74	Joback Method
cpg	151.74	J/mol×K	476.01	Joback Method
cpg	157.89	J/mol×K	507.27	Joback Method

cpg	163.76	J/mol×K	538.53	Joback Method
cpg	169.37	J/mol×K	569.79	Joback Method
dvisc	0.0034502	Pa×s	214.69	Joback Method
dvisc	0.0019085	Pa×s	242.61	Joback Method
dvisc	0.0011929	Pa×s	270.53	Joback Method
dvisc	0.0008142	Pa×s	298.46	Joback Method
dvisc	0.0005932	Pa×s	326.38	Joback Method
dvisc	0.0004543	Pa×s	354.30	Joback Method
dvisc	0.0003618	Pa×s	382.22	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	326.00 ± 2.00	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
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=C6322492&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

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

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