1-Chloropentan-2-one

Inchi: InChI=1S/C5H9ClO/c1-2-3-5(7)4-6/h2-4H2,1H3
InchiKey: MGTGUEKJBFTQQW-UHFFFAOYSA-N
Formula: C5H9ClO
SMILES: CCCC(=O)CCl
Mol. weight [g/mol]: 120.58

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
rinpol	851.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	878.00		NIST Webbook
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

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=R632861&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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