2-Pentanone, 3-chloro-

Other names: 3-chloropentan-2-one
Inchi: InChI=1S/C5H9ClO/c1-3-5(6)4(2)7/h5H,3H2,1-2H3
InchiKey: CKSIBFLEDRJUTN-UHFFFAOYSA-N
Formula: C5H9ClO
SMILES: CCC(Cl)C(C)=O
Mol. weight [g/mol]: 120.58
CAS: 13280-00-7

Physical Properties

Property code	Value	Unit	Source
gf	-152.07	kJ/mol	Joback Method
hf	-280.13	kJ/mol	Joback Method
hfus	10.98	kJ/mol	Joback Method
hvap	37.47	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.593		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinpol	850.00		NIST Webbook
rinpol	795.00		NIST Webbook
tb	404.66	K	Joback Method
tc	595.49	K	Joback Method
tf	210.96	K	Joback Method
vc	0.364	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.21	J/mol×K	404.66	Joback Method
cpg	206.34	J/mol×K	563.69	Joback Method
cpg	199.04	J/mol×K	531.88	Joback Method
cpg	191.40	J/mol×K	500.08	Joback Method
cpg	183.38	J/mol×K	468.27	Joback Method
cpg	174.99	J/mol×K	436.47	Joback Method

cpg	213.28	J/mol×K	595.49	Joback Method
dvisc	0.0003464	Pa×s	404.66	Joback Method
dvisc	0.0004515	Pa×s	372.38	Joback Method
dvisc	0.0006188	Pa×s	340.09	Joback Method
dvisc	0.0009061	Pa×s	307.81	Joback Method
dvisc	0.0014508	Pa×s	275.53	Joback Method
dvisc	0.0026320	Pa×s	243.24	Joback Method
dvisc	0.0057299	Pa×s	210.96	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13280007&Units=SI
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

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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