3-Heptanone, 4-chloro

Inchi: InChI=1S/C7H13ClO/c1-3-5-6(8)7(9)4-2/h6H,3-5H2,1-2H3
InchiKey: KGXLUVXAXCJDPO-UHFFFAOYSA-N
Formula: C7H13ClO
SMILES: CCCC(Cl)C(=O)CC
Mol. weight [g/mol]: 148.63

Physical Properties

Property code	Value	Unit	Source
gf	-135.23	kJ/mol	Joback Method
hf	-321.41	kJ/mol	Joback Method
hfus	16.16	kJ/mol	Joback Method
hvap	41.92	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.373		Crippen Method
mcvol	123.300	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
rinpol	982.00		NIST Webbook
rinpol	982.00		NIST Webbook
tb	450.42	K	Joback Method
tc	637.88	K	Joback Method
tf	233.50	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.58	J/mol×K	450.42	Joback Method
cpg	253.92	J/mol×K	481.66	Joback Method
cpg	264.75	J/mol×K	512.91	Joback Method
cpg	275.09	J/mol×K	544.15	Joback Method
cpg	284.95	J/mol×K	575.40	Joback Method
cpg	294.35	J/mol×K	606.64	Joback Method
cpg	303.29	J/mol×K	637.88	Joback Method
dvisc	0.0060348	Pa×s	233.50	Joback Method

dvisc	0.0026628	Pa×s	269.65	Joback Method
dvisc	0.0014257	Pa×s	305.81	Joback Method
dvisc	0.0008712	Pa×s	341.96	Joback Method
dvisc	0.0005849	Pa×s	378.11	Joback Method
dvisc	0.0004210	Pa×s	414.27	Joback Method
dvisc	0.0003194	Pa×s	450.42	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R630132&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