

4-Heptanone, 3-chloro

Inchi:	InChI=1S/C7H13ClO/c1-3-5-7(9)6(8)4-2/h6H,3-5H2,1-2H3
InchiKey:	ONHHYBUXHMRHFZ-UHFFFAOYSA-N
Formula:	C7H13ClO
SMILES:	CCCC(=O)C(Cl)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
rinpola	977.00		NIST Webbook
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tb	450.42	K	Joback Method
tc	637.88	K	Joback Method
tf	233.50	K	Joback Method
vc	0.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.58	J/molxK	450.42	Joback Method
cpg	294.35	J/molxK	606.64	Joback Method
cpg	284.95	J/molxK	575.40	Joback Method
cpg	275.09	J/molxK	544.15	Joback Method
cpg	264.75	J/molxK	512.91	Joback Method
cpg	253.92	J/molxK	481.66	Joback Method
cpg	303.29	J/molxK	637.88	Joback Method
dvisc	0.0003194	Paxs	450.42	Joback Method

dvisc	0.0004210	Paxs	414.27	Joback Method
dvisc	0.0005849	Paxs	378.11	Joback Method
dvisc	0.0008712	Paxs	341.96	Joback Method
dvisc	0.0014257	Paxs	305.81	Joback Method
dvisc	0.0026628	Paxs	269.65	Joback Method
dvisc	0.0060348	Paxs	233.50	Joback Method

Sources

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=R630578&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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