3-chlorononane

Other names: Nonane, 3-chloro-
Inchi: InChI=1S/C9H19Cl/c1-3-5-6-7-8-9(10)4-2/h9H,3-8H2,1-2H3
InchiKey: ASQUFLQVFQDUFF-UHFFFAOYSA-N
Formula: C9H19Cl
SMILES: CCCCCCC(Cl)CC
Mol. weight [g/mol]: 162.70
CAS: 28123-68-4

Physical Properties

Property code	Value	Unit	Source
gf	10.53	kJ/mol	Joback Method
hf	-250.11	kJ/mol	Joback Method
hfus	19.74	kJ/mol	Joback Method
hvap	39.62	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.974		Crippen Method
mcvol	149.910	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
ripol	1264.00		NIST Webbook
ripol	1264.00		NIST Webbook
tb	442.31	K	Joback Method
tc	615.85	K	Joback Method
tf	206.11	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.70	J/mol×K	442.31	Joback Method
cpg	318.86	J/mol×K	471.23	Joback Method
cpg	332.46	J/mol×K	500.16	Joback Method

cpg	345.50	J/mol×K	529.08	Joback Method
cpg	357.99	J/mol×K	558.00	Joback Method
cpg	369.96	J/mol×K	586.93	Joback Method
cpg	381.42	J/mol×K	615.85	Joback Method
dvisc	0.0087685	Pa×s	206.11	Joback Method
dvisc	0.0030269	Pa×s	245.48	Joback Method
dvisc	0.0014020	Pa×s	284.84	Joback Method
dvisc	0.0007828	Pa×s	324.21	Joback Method
dvisc	0.0004959	Pa×s	363.58	Joback Method
dvisc	0.0003434	Pa×s	402.94	Joback Method
dvisc	0.0002539	Pa×s	442.31	Joback Method

Sources

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=C28123684&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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