Nonane, 3-chloro-

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

Physical Properties

Property code	Value	Unit	Source
af	0.4499		Cheméo Relay (1.0)
gf	10.53	kJ/mol	Joback Method
hf	-262.79	kJ/mol	Cheméo Relay (1.0)
hfus	19.74	kJ/mol	Joback Method
hvap	51.18	kJ/mol	Cheméo Relay (1.0)
ie	9.99	eV	Cheméo Relay (1.0)
log10ws	-4.97		Cheméo Relay (1.0)
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	456.00	K	Cheméo Relay (1.0)
tc	641.41	K	Cheméo Relay (1.0)
tf	218.49	K	Cheméo Relay (1.0)
vc	0.570	m3/kmol	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28123684&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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