

NONADECANE, 1-CHLORO-

Other names:	1-Chloro nonadecane
Inchi:	InChI=1S/C19H39Cl/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20/h2-19H2,1H3
InchiKey:	ZPHKHTAJPZOPHM-UHFFFAOYSA-N
Formula:	C19H39Cl
SMILES:	CCCCCCCCCCCCCCCCCCCCI
Mol. weight [g/mol]:	302.97

Physical Properties

Property code	Value	Unit	Source
af	0.8743		Cheméo Relay (1.0)
gf	97.17	kJ/mol	Joback Method
hf	-480.82	kJ/mol	Cheméo Relay (1.0)
hfus	49.16	kJ/mol	Joback Method
hvap	114.70	kJ/mol	NIST Webbook
ie	10.29	eV	Cheméo Relay (1.0)
log10ws	-8.39		Cheméo Relay (1.0)
logp	7.877		Crippen Method
mcvol	290.810	ml/mol	McGowan Method
pc	1054.83	kPa	Joback Method
rinpol	360.90		NIST Webbook
rinpol	360.90		NIST Webbook
tb	580.75	K	Cheméo Relay (1.0)
tc	771.27	K	Cheméo Relay (1.0)
tf	315.44	K	Cheméo Relay (1.0)
vc	1.166	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.58	J/mol×K	808.88	Joback Method
cpg	927.38	J/mol×K	836.35	Joback Method
cpg	840.75	J/mol×K	699.02	Joback Method
cpg	859.66	J/mol×K	726.48	Joback Method
cpg	877.75	J/mol×K	753.95	Joback Method

cpg	895.04	J/mol×K	781.42	Joback Method
cpg	821.00	J/mol×K	671.55	Joback Method
dvisc	0.0005441	Pa×s	446.39	Joback Method
dvisc	0.0011337	Pa×s	390.10	Joback Method
dvisc	0.0030255	Pa×s	333.81	Joback Method
dvisc	0.0003078	Pa×s	502.68	Joback Method
dvisc	0.0001953	Pa×s	558.97	Joback Method
dvisc	0.0001347	Pa×s	615.26	Joback Method
dvisc	0.0000988	Pa×s	671.55	Joback Method
hvapt	76.30	kJ/mol	578.00	NIST Webbook

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=C62016766&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
hvapt:	Enthalpy of vaporization at a given temperature
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
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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