

Decane, 1-chloro-

Other names:	1-Chlorodecane Decyl chloride n-Decyl chloride
Inchi:	InChI=1S/C10H21Cl/c1-2-3-4-5-6-7-8-9-10-11/h2-10H2,1H3
InchiKey:	ZTEHOZMYMCEYRM-UHFFFAOYSA-N
Formula:	C10H21Cl
SMILES:	CCCCCCCCCCCCI
Mol. weight [g/mol]:	176.73
CAS:	1002-69-3

Physical Properties

Property code	Value	Unit	Source
gf	21.39	kJ/mol	Joback Method
hf	-265.47	kJ/mol	Joback Method
hfus	25.85	kJ/mol	Joback Method
hvap	64.00 ± 0.20	kJ/mol	NIST Webbook
log10ws	-4.16		Crippen Method
logp	4.366		Crippen Method
mcvol	164.000	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	1254.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1264.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1249.60		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1249.60		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1261.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1452.00		NIST Webbook
ripol	1455.00		NIST Webbook
ripol	1459.00		NIST Webbook

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ripol	1452.00		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	1469.00		NIST Webbook
ripol	1468.00		NIST Webbook
ripol	1470.00		NIST Webbook
tb	495.65 ± 1.50	K	NIST Webbook
tb	496.40 ± 1.50	K	NIST Webbook
tb	496.60	K	NIST Webbook
tc	634.39	K	Joback Method
tf	232.38	K	Joback Method
vc	0.644	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.27	J/mol×K	493.76	Joback Method
cpg	428.35	J/mol×K	634.39	Joback Method
cpg	416.41	J/mol×K	606.27	Joback Method
cpg	403.94	J/mol×K	578.14	Joback Method
cpg	390.94	J/mol×K	550.01	Joback Method
cpg	377.38	J/mol×K	521.88	Joback Method
cpg	348.57	J/mol×K	465.63	Joback Method
cpl	346.36	J/mol×K	321.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis

cpl	355.52	J/molxK	339.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	352.76	J/molxK	334.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	351.31	J/molxK	331.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	350.01	J/molxK	329.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis

cpl	348.75	J/molxK	326.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	356.17	J/molxK	341.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	346.99	J/molxK	324.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	357.74	J/molxK	344.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis

cpl	358.38	J/molxK	346.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	359.65	J/molxK	349.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	361.49	J/molxK	351.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	362.49	J/molxK	353.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis

cpl	328.57	J/molxK	284.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	329.82	J/molxK	286.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	331.00	J/molxK	289.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	332.01	J/molxK	291.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis

cpl	333.14	J/mol×K	294.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	334.13	J/mol×K	296.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	335.39	J/mol×K	299.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	336.61	J/mol×K	301.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis

cpl	337.47	J/mol×K	304.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	338.66	J/mol×K	306.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	339.83	J/mol×K	309.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	341.39	J/mol×K	311.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis

cpl	342.42	J/molxK	314.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	343.41	J/molxK	316.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	345.04	J/molxK	319.15	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
cpl	353.39	J/molxK	336.65	Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 284.15 K to 353.15 K. A group additivity and molecular connectivity analysis
dvisc	0.0022338	Paxs	271.25	Joback Method
dvisc	0.0003301	Paxs	426.75	Joback Method
dvisc	0.0004612	Paxs	387.88	Joback Method
dvisc	0.0006940	Paxs	349.00	Joback Method
dvisc	0.0011571	Paxs	310.13	Joback Method
dvisc	0.0002499	Paxs	465.63	Joback Method

dvisc	0.0053737	Paxs	232.38	Joback Method
hvapt	54.40	kJ/mol	454.50	NIST Webbook
hvapt	56.20	kJ/mol	429.00	NIST Webbook
rhoI	892.30	kg/m3	263.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhoI	884.20	kg/m3	273.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhoI	899.90	kg/m3	253.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhoI	876.80	kg/m3	283.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhoI	868.90	kg/m3	293.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhoI	845.60	kg/m3	323.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhoI	830.00	kg/m3	343.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhoI	814.20	kg/m3	363.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K

rhoI	789.50	kg/m3	393.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhoI	764.60	kg/m3	423.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K
rhoI	865.00	kg/m3	298.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.58375e+01
Coeff. B	-4.67024e+03
Coeff. C	-7.98780e+01
Temperature range (K), min.	380.22
Temperature range (K), max.	523.56

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature range from 253.15 to 423.15 K:	https://www.doi.org/10.1021/je049652j
Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K:	https://www.doi.org/10.1021/je700325c
Connectivity analysis:	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=C1002693&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rho:	Liquid Density
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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