Decane, 1-chloro-

Other names: 1-Chlorodecane

Decyl chloride

n-Decyl chloride

InChl=1S/C10H21Cl/c1-2-3-4-5-6-7-8-9-10-11/h2-10H2,1H3

InchiKey: ZTEHOZMYMCEYRM-UHFFFAOYSA-N

Formula: C10H21Cl

SMILES: CCCCCCCCCI

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
рс	2038.23	kPa	Joback Method
rinpol	1275.00		NIST Webbook
rinpol	1263.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1256.00		NIST Webbook
rinpol	1261.00		NIST Webbook
rinpol	1255.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1249.60		NIST Webbook
rinpol	1275.00		NIST Webbook
rinpol	1254.00		NIST Webbook
rinpol	1249.60		NIST Webbook
rinpol	1264.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1452.00		NIST Webbook
ripol	1455.00		NIST Webbook
ripol	1459.00		NIST Webbook
ripol	1459.00		NIST Webbook

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
ripol	1474.00		NIST Webbook
tb	496.60	K	NIST Webbook
tb	496.40 ± 1.50	K	NIST Webbook
tb	495.65 ± 1.50	K	NIST Webbook
tc	634.39	K	Joback Method
tf	232.38	K	Joback Method
VC	0.644	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.35	J/mol×K	634.39	Joback Method
cpg	363.27	J/mol×K	493.76	Joback Method
cpg	377.38	J/mol×K	521.88	Joback Method
cpg	390.94	J/mol×K	550.01	Joback Method
cpg	403.94	J/mol×K	578.14	Joback Method
cpg	416.41	J/mol×K	606.27	Joback Method
cpg	348.57	J/mol×K	465.63	Joback Method
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/mol×K	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/mol×K	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/mol×K	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	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	346.99	J/mol×K	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	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	350.01	J/mol×K	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	351.31	J/mol×K	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	352.76	J/mol×K	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	353.39	J/mol×K	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	
cpl	355.52	J/mol×K	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	356.17	J/mol×K	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	357.74	J/mol×K	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/mol×K	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/mol×K	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/mol×K	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/mol×K	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	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	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	332.01	J/mol×K	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	331.00	J/mol×K	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	329.82	J/mol×K	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	348.75	J/mol×K	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	328.57	J/mol×K	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	
dvisc	0.0004612	Paxs	387.88	Joback Method	
			400.75	Joback Method	
dvisc	0.0003301	Paxs	426.75	JUDACK MICHIOU	
	0.0003301 0.0053737	Paxs Paxs	232.38	Joback Method	
dvisc					
dvisc dvisc	0.0053737	Paxs	232.38	Joback Method	

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dvisc	0.0002499	Paxs	465.63	Joback Method	
hvapt	54.40	kJ/mol	454.50	NIST Webbook	
hvapt	56.20	kJ/mol	429.00	NIST Webbook	
rhol	814.20	kg/m3	363.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K	
rhol	830.00	kg/m3	343.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K	
rhol	789.50	kg/m3	393.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K	
rhol	845.60	kg/m3	323.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K	
rhol	865.00	kg/m3	298.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K	
rhol	868.90	kg/m3	293.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K	
rhol	876.80	kg/m3	283.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K	
rhol	884.20	kg/m3	273.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K	

rhol	892.30	kg/m3	263.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K	
rhol	899.90	kg/m3	253.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K	
rhol	764.60	kg/m3	423.15	Density of Some 1-Chloroalkanes within the Temperature Range from (253.15 to 423.15) K	

Correlations

Information Value

Property code	pvap
Equation	ln(Pvp) = 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

http://link.springer.com/article/10.1007/BF02311772 McGowan Method:

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1002693&Units=SI

The Yaws Handbook of Vapor https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure Pressure: Crippen Method:

http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Heat Capacities of 1-chloroalkanes and 1-bromoalkanes within the temperature Panaity of State of State

https://www.doi.org/10.1021/je700325c https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacitycpl: Liquid phase heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formationhf: Enthalpy of formation at standard conditionshfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditionshvapt: Enthalpy of vaporization at a given temperature

log10ws: Log10 of Water solubility in mol/llogp: Octanol/Water partition coefficientmcvol: McGowan's characteristic volume

pc: Critical Pressurepvap: Vapor pressurerhol: 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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