Dodecane, 1-chloro-

Other names:	1-Chlorododecane
	Dodecyl chloride
	Lauryl chloride
	n-Dodecyl chloride
Inchi:	InChI=1S/C12H25Cl/c1-2-3-4-5-6-7-8-9-10-11-12-13/h2-12H2,1H3
InchiKey:	YAYNEUUHHLGGAH-UHFFFAOYSA-N
Formula:	C12H25Cl
SMILES:	CCCCCCCCCCCCCl
Mol. weight [g/mol]:	204.78
CAS:	112-52-7

Physical Properties

Property code	Value	Unit	Source
chl	-7926.40 ± 2.40	kJ/mol	NIST Webbook
gf	38.23	kJ/mol	Joback Method
hf	-322.00 ± 2.50	kJ/mol	NIST Webbook
hfl	-392.30 ± 2.40	kJ/mol	NIST Webbook
hfus	31.03	kJ/mol	Joback Method
hvap	70.30 ± 0.50	kJ/mol	NIST Webbook
hvap	71.90 ± 0.30	kJ/mol	NIST Webbook
hvap	71.93 ± 0.32	kJ/mol	NIST Webbook
hvap	73.90 ± 1.40	kJ/mol	NIST Webbook
hvap	75.80	kJ/mol	NIST Webbook
hvap	71.13	kJ/mol	NIST Webbook
hvap	70.50	kJ/mol	NIST Webbook
log10ws	-5.00		Crippen Method
logp	5.146		Crippen Method
mcvol	192.180	ml/mol	McGowan Method
pc	1726.03	kPa	Joback Method
rinpol	1469.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1469.00		NIST Webbook
rinpol	1461.00		NIST Webbook
rinpol	246.60		NIST Webbook
rinpol	246.60		NIST Webbook
rinpol	1432.00		NIST Webbook
ripol	1664.00		NIST Webbook

ripol	1684.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1661.00		NIST Webbook
tb	533.20	K	NIST Webbook
tc	677.96	K	Joback Method
tf	254.92	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.27	J/mol×K	677.96	Joback Method
cpg	517.11	J/mol×K	650.20	Joback Method
cpg	503.37	J/mol×K	622.44	Joback Method
cpg	489.03	J/mol×K	594.68	Joback Method
cpg	474.08	J/mol×K	566.91	Joback Method
cpg	458.49	J/mol×K	539.15	Joback Method
cpg	442.26	J/mol×K	511.39	Joback Method
dvisc	0.0050937	Pa×s	254.92	Joback Method
dvisc	0.0002138	Pa×s	511.39	Joback Method
dvisc	0.0002850	Pa×s	468.64	Joback Method
dvisc	0.0004025	Pa×s	425.90	Joback Method
dvisc	0.0006139	Pa×s	383.15	Joback Method
dvisc	0.0010411	Pa×s	340.41	Joback Method
dvisc	0.0020547	Pa×s	297.67	Joback Method
hvapt	62.40	kJ/mol	454.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.60	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58353e+01
Coeff. B	-4.97239e+03
Coeff. C	-9.02500e+01
Temperature range (K), min.	410.06
Temperature range (K), max.	562.74

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C112527&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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