1-Chloroundecane

Other names: Undecane, 1-chloro-
Undecyl chloride
n-Undecyl chloride
Inchi: InChI=1S/C11H23Cl/c1-2-3-4-5-6-7-8-9-10-11-12/h2-11H2,1H3
InchiKey: ZHKKNUKCXPWZOP-UHFFFAOYSA-N
Formula: C11H23Cl
SMILES: CCCCCCCCCCCCl
Mol. weight [g/mol]: 190.75
CAS: 2473-03-2

Physical Properties

Property code	Value	Unit	Source
gf	29.81	kJ/mol	Joback Method
hf	-286.11	kJ/mol	Joback Method
hfus	28.44	kJ/mol	Joback Method
hvap	65.90	kJ/mol	NIST Webbook
hvap	70.20	kJ/mol	NIST Webbook
log10ws	-4.58		Crippen Method
logp	4.756		Crippen Method
mcvol	178.090	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinpol	1358.00		NIST Webbook
rinpol	1365.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1561.00		NIST Webbook
tb	488.51	K	Joback Method
tc	656.16	K	Joback Method
tf	243.65	K	Joback Method
vc	0.701	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	394.47	J/mol×K	488.51	Joback Method
cpg	409.99	J/mol×K	516.45	Joback Method
cpg	424.88	J/mol×K	544.39	Joback Method
cpg	439.17	J/mol×K	572.33	Joback Method
cpg	452.88	J/mol×K	600.28	Joback Method
cpg	466.03	J/mol×K	628.22	Joback Method
cpg	478.62	J/mol×K	656.16	Joback Method
dvisc	0.0052700	Pa×s	243.65	Joback Method
dvisc	0.0021565	Pa×s	284.46	Joback Method
dvisc	0.0011043	Pa×s	325.27	Joback Method
dvisc	0.0006564	Pa×s	366.08	Joback Method
dvisc	0.0004331	Pa×s	406.89	Joback Method
dvisc	0.0003083	Pa×s	447.70	Joback Method
dvisc	0.0002323	Pa×s	488.51	Joback Method
hvapt	59.40	kJ/mol	446.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55784e+01
Coeff. B	-4.74781e+03
Coeff. C	-8.52900e+01
Temperature range (K), min.	395.79
Temperature range (K), max.	547.73

Sources

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=C2473032&Units=SI

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

Legend

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