Ethyl Chloride

Other names:	Aethylchlorid
	Aethylis
	Aethylis chloridum
	Anodynon
	C2H5Cl
	Chelen
	Chloorethaan
	Chlorene
	Chlorethyl
	Chloridum
	Chloroaethan
	Chloroethane
	Chlorure D'ethyle
	Chloryl
	Chloryl anesthetic
	Chloryle anesthetic
	Cloretilo
	Cloroetano
	Cloruro di etile
	Dublofix
	Ethane, chloro-
	Ether chloratus
	Ether hydrochloric
	Ether muriatic
	Etylu chlorek
	Hydrochloric ether
	Kelene
	Monochlorethane
	Monochloroethane
	Muriatic ether
	NCI-C06224
	Narcotile
	R-160
	UN 1037
	freon 160
Inchi:	InChI=1S/C2H5Cl/c1-2-3/h2H2,1H3
InchiKey:	HRYZWHHZPQKTII-UHFFFAOYSA-N
Formula:	C2H5Cl
SMILES:	CCCl
Mol. weight [g/mol]:	64.51

CAS: 75-00-3

Physical Properties

Property code	Value	Unit	Source
af	0.1910		KDB
affp	693.40	kJ/mol	NIST Webbook
affp	679.50 ± 1.40	kJ/mol	NIST Webbook
aigt	792.04	K	KDB
basg	666.90	kJ/mol	NIST Webbook
basg	655.60 ± 1.40	kJ/mol	NIST Webbook
chg	-1430.00 ± 10.00	kJ/mol	NIST Webbook
chg	-1413.10 ± 0.59	kJ/mol	NIST Webbook
dm	2.00	debye	KDB
ep	28.50	J/mol×K	NIST Webbook
fll	3.60	% in Air	KDB
flu	12.00	% in Air	KDB
fpc	230.37	K	KDB
fpo	223.15	K	KDB
gf	-60.04	kJ/mol	KDB
hf	-100.00	kJ/mol	NIST Webbook
hf	-112.30 ± 0.75	kJ/mol	NIST Webbook
hf	-109.00 ± 2.00	kJ/mol	NIST Webbook
hf	-112.10 ± 0.70	kJ/mol	NIST Webbook
hf	-111.80	kJ/mol	KDB
hf	-112.00	kJ/mol	NIST Webbook
hf	-107.70 ± 0.59	kJ/mol	NIST Webbook
hfl	-137.00 ± 1.00	kJ/mol	NIST Webbook
hfus	5.13	kJ/mol	Joback Method
hvap	24.60 ± 0.30	kJ/mol	NIST Webbook
ie	11.01	eV	NIST Webbook
ie	10.95	eV	NIST Webbook
ie	10.98 ± 0.02	eV	NIST Webbook
ie	11.04 ± 0.05	eV	NIST Webbook
ie	11.06	eV	NIST Webbook
ie	11.01	eV	NIST Webbook
ie	11.00	eV	NIST Webbook
ie	11.06 ± 0.02	eV	NIST Webbook
ie	10.98 ± 0.02	eV	NIST Webbook
ie	11.01	eV	NIST Webbook
ie	10.97 ± 0.02	eV	NIST Webbook

ie	10.98 ± 0.01	eV	NIST Webbook
log10ws	-1.06		Aqueous Solubility Prediction Method
log10ws	-1.06		Estimated Solubility Method
logp	1.245		Crippen Method
mcvol	51.280	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=2)		KDB
pc	5240.53 ± 40.53	kPa	NIST Webbook
pc	5300.00	kPa	KDB
rinpol	431.00		NIST Webbook
rinpol	427.00		NIST Webbook
rinpol	432.00		NIST Webbook
rinpol	423.96		NIST Webbook
rinpol	424.09		NIST Webbook
rinpol	424.00		NIST Webbook
rinpol	455.00		NIST Webbook
rinpol	430.00		NIST Webbook
rinpol	417.00		NIST Webbook
rinpol	446.00		NIST Webbook
rinpol	432.00		NIST Webbook
rinpol	430.00		NIST Webbook
rinpol	430.00		NIST Webbook
rinpol	430.00		NIST Webbook
rinpol	426.00		NIST Webbook
rinpol	430.00		NIST Webbook
rinpol	432.00		NIST Webbook
rinpol	426.00		NIST Webbook
rinpol	447.00		NIST Webbook
rinpol	447.00		NIST Webbook
rinpol	441.00		NIST Webbook
rinpol	414.00		NIST Webbook
rinpol	416.00		NIST Webbook
rinpol	430.00		NIST Webbook
rinpol	455.00		NIST Webbook
rinpol	415.00		NIST Webbook
rinpol	414.00		NIST Webbook
rinpol	416.00		NIST Webbook
rinpol	431.00		NIST Webbook
rinpol	431.00		NIST Webbook
rinpol	441.00		NIST Webbook
rinpol	432.00		NIST Webbook
rinpol	434.00		NIST Webbook
ripol	668.00		NIST Webbook

ripol	668.00		NIST Webbook
ripol	661.08		NIST Webbook
ripol	661.45		NIST Webbook
ripol	661.48		NIST Webbook
ripol	668.00		NIST Webbook
sl	186.27	J/mol×K	NIST Webbook
tb	286.00 ± 0.50	K	NIST Webbook
tb	285.45 ± 0.20	K	NIST Webbook
tb	286.25 ± 0.60	K	NIST Webbook
tb	286.05 ± 0.50	K	NIST Webbook
tb	287.10 ± 0.30	K	NIST Webbook
tb	285.50	K	NIST Webbook
tb	286.20	K	KDB
tb	307.90 ± 0.70	K	NIST Webbook
tb	287.20 ± 0.20	K	NIST Webbook
tc	460.35 ± 0.40	K	NIST Webbook
tc	460.40	K	KDB
tf	133.00 ± 2.00	K	NIST Webbook
tf	137.00 ± 0.50	K	NIST Webbook
tf	132.30 ± 0.20	K	NIST Webbook
tf	134.30	K	Aqueous Solubility Prediction Method
tf	134.40	K	KDB
tf	136.75 ± 0.40	K	NIST Webbook
tt	134.82 ± 0.02	K	NIST Webbook
vc	0.199	m3/kmol	KDB
zc	0.2755220		KDB
zra	0.27		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	62.72	J/mol×K	282.59	Joback Method
cpg	81.78	J/mol×K	424.44	Joback Method
cpg	78.23	J/mol×K	396.07	Joback Method
cpg	74.55	J/mol×K	367.70	Joback Method
cpg	70.74	J/mol×K	339.33	Joback Method
cpg	66.80	J/mol×K	310.96	Joback Method
cpg	85.20	J/mol×K	452.81	Joback Method
cpl	103.30	J/mol×K	290.00	NIST Webbook
cpl	107.70	J/mol×K	298.00	NIST Webbook

cpl	108.80	J/mol×K	298.00	NIST Webbook
cpl	109.60	J/mol×K	288.00	NIST Webbook
cpl	108.80	J/mol×K	298.10	NIST Webbook
dvisc	0.0002797	Pa×s	259.20	Joback Method
dvisc	0.0002258	Pa×s	282.59	Joback Method
dvisc	0.0003615	Pa×s	235.80	Joback Method
dvisc	0.0004943	Pa×s	212.41	Joback Method
dvisc	0.0007304	Pa×s	189.01	Joback Method
dvisc	0.0012052	Pa×s	165.62	Joback Method
dvisc	0.0023449	Pa×s	142.22	Joback Method
hfust	4.45	kJ/mol	134.80	NIST Webbook
hfust	4.45	kJ/mol	134.80	NIST Webbook
hfust	4.45	kJ/mol	134.82	NIST Webbook
hvapt	24.40	kJ/mol	431.50	NIST Webbook
hvapt	24.40	kJ/mol	373.50	NIST Webbook
hvapt	27.80	kJ/mol	256.00	NIST Webbook
hvapt	25.90	kJ/mol	251.50	NIST Webbook
hvapt	24.83	kJ/mol	294.00	NIST Webbook
hvapt	25.10	kJ/mol	314.50	NIST Webbook
hvapt	24.65	kJ/mol	285.42	NIST Webbook
hvapt	24.69	kJ/mol	285.50	KDB
rhol	896.00	kg/m3	293.00	KDB
sfust	33.02	J/mol×K	134.82	NIST Webbook
srf	0.02	N/m	283.20	KDB
svapt	86.37	J/mol×K	285.42	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39805e+01
Coeff. B	-2.45158e+03
Coeff. C	-2.71410e+01
Temperature range (K), min.	206.18
Temperature range (K), max.	460.35

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	6.25703e+01
Coeff. B	-4.77239e+03
Coeff. C	-7.41963e+00
Coeff. D	8.84845e-06
Temperature range (K), min.	136.75
Temperature range (K), max.	460.35

Sources

Henry's Law Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, 2-Methylpropene, trans-2-Butene, cis-2-Butene, 1,3-Butadiene, Dimethyl Ether, Chloroethane, and 1,1-Difluoroethane in Methanol:	https://www.doi.org/10.1021/je100529s
Henry's law constants and infinite dilution activity coefficients of Joback Method, Diethylether, 2-Methylpropene, trans-2-Butene, cis-2-Butene, 1,3-Butadiene, Dimethyl Ether, Chloroethane, and 1,1-Difluoroethane in 1-propanol, 2-propanol, 1-butanol, 2-butanol, isobutanol, 2-methyl-1-butanol, and 3-methyl-1-butanol:	https://www.doi.org/10.1016/j.jct.2005.08.004
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.org/cgi/cbook.cgi?ID=C75003&Units=SI
Henry's Law Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, 2-Methylpropene, trans-2-Butene, cis-2-Butene, 1,3-Butadiene, Dimethyl Ether, Chloroethane, and 1,1-Difluoroethane in 2-Methyl-3-buten-2-ol and 3-Methyl-3-buten-1-ol:	https://www.doi.org/10.1021/je050343i
Yaws Handbook Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
IDDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1578
Henry's Law Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, 2-Methylpropane, 1-Butene, 2-Methylpropene, trans-2-Butene, cis-2-Butene, 1,3-Butadiene, Dimethylether, Chloroethane, 1,1-Difluoroethane, and Hexane in Tetrahydropyran:	https://www.doi.org/10.1021/je700270d
Determination of Henry's Law Constants Using Internal Standards and Estimated Solubility Method:	https://www.doi.org/10.1021/je3010535
Chiappe Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Henry's Law Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, 2-Methylpropane, 1-Butene, 2-Methylpropene, trans-2-Butene, cis-2-Butene, 1,3-Butadiene, Dimethyl Ether, Chloroethane, and 1,1-Difluoroethane in 2-Propen-1-ol:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.doi.org/10.1021/je0502647
Henry's Law Constants and Infinite Dilution Activity Coefficients of Propane, Propene, Butane, 2-Methylpropane, 1-Butene, 2-Methylpropene, trans-2-Butene, cis-2-Butene, 1,3-Butadiene, Dimethyl Ether, Chloroethane, and 1,1-Difluoroethane in Benzene, Toluene, o-Xylene, m-Xylene, p-Xylene, and Styrene:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1578
	https://www.doi.org/10.1021/je060395n

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
chg:	Standard gas enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dm:	Dipole Moment
dvisc:	Dynamic viscosity
ep:	Protonation entropy at 298K

fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpc:	Flash Point (Closed Cup Method)
fpo:	Flash Point (Open Cup Method)
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
hfust:	Enthalpy of fusion at a given temperature
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
srf:	Surface Tension
svapt:	Entropy of vaporization at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility
zra:	Rackett Parameter