Benzene, 1-chloro-4-ethoxy-

Other names:	1-Chloro-4-ethoxybenzene
	4-Chlorophenetole
	4-Chlorophenol ethyl ether
	NSC 6161
	Phenetole, p-chloro-
	p-Chlorophenetole
	p-Chlorophenyl ethyl ether
	p-Ethoxychlorobenzene
Inchi:	InChI=1S/C8H9ClO/c1-2-10-8-5-3-7(9)4-6-8/h3-6H,2H2,1H3
InchiKey:	IXLSVQMYQRAMEW-UHFFFAOYSA-N
Formula:	C8H9ClO
SMILES:	CCOc1ccc(Cl)cc1
Mol. weight [g/mol]:	156.61
CAS:	622-61-7

Physical Properties

Property code	Value	Unit	Source
gf	2.33	kJ/mol	Joback Method
hf	-131.35	kJ/mol	Joback Method
hfus	15.51	kJ/mol	Joback Method
hvap	43.14	kJ/mol	Joback Method
ie	8.46 ± 0.15	eV	NIST Webbook
log10ws	-2.69		Crippen Method
logp	2.739		Crippen Method
mcvol	117.930	ml/mol	McGowan Method
pc	3364.54	kPa	Joback Method
rinpol	1157.60		NIST Webbook
rinpol	1157.60		NIST Webbook
tb	485.09 ± 0.07	K	NIST Webbook
tc	690.26	K	Joback Method
tf	290.29 ± 0.05	K	NIST Webbook
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.21	J/mol×K	473.95	Joback Method
cpg	235.63	J/mol×K	510.00	Joback Method
cpg	246.47	J/mol×K	546.05	Joback Method
cpg	256.73	J/mol×K	582.10	Joback Method
cpg	266.42	J/mol×K	618.15	Joback Method
cpg	275.56	J/mol×K	654.20	Joback Method
cpg	284.16	J/mol×K	690.26	Joback Method
dvisc	0.0018210	Pa×s	271.01	Joback Method
dvisc	0.0010524	Pa×s	304.83	Joback Method
dvisc	0.0006786	Pa×s	338.66	Joback Method
dvisc	0.0004738	Pa×s	372.48	Joback Method
dvisc	0.0003513	Pa×s	406.30	Joback Method
dvisc	0.0002727	Pa×s	440.13	Joback Method
dvisc	0.0002194	Pa×s	473.95	Joback Method
hvapt	49.50	kJ/mol	440.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48433e+01
Coeff. B	-4.57835e+03
Coeff. C	-4.31500e+01
Temperature range (K), min.	357.69
Temperature range (K), max.	523.47

Sources

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=C622617&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume