Benzene, 1-chloro-3-ethyl-

Other names: 1-Chloro-3-ethylbenzene
3-Ethylchlorobenzene
m-Chloroethylbenzene
Inchi: InChI=1S/C8H9Cl/c1-2-7-4-3-5-8(9)6-7/h3-6H,2H2,1H3
InchiKey: LOXUEGMPESDGBQ-UHFFFAOYSA-N
Formula: C8H9Cl
SMILES: CCc1cccc(Cl)c1
Mol. weight [g/mol]: 140.61
CAS: 620-16-6

Physical Properties

Property code	Value	Unit	Source
gf	107.33	kJ/mol	Joback Method
hf	0.87	kJ/mol	Joback Method
hfl	-50.71	kJ/mol	NIST Webbook
hfus	14.32	kJ/mol	Joback Method
hvap	40.73	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	2.902		Crippen Method
mcvol	112.060	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
rinpol	1036.00		NIST Webbook
tb	457.00	K	NIST Webbook
tb	457.15 ± 1.50	K	NIST Webbook
tb	456.92 ± 0.07	K	NIST Webbook
tc	669.70	K	Joback Method
tf	218.11 ± 0.05	K	NIST Webbook
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	202.26	J/mol×K	451.53	Joback Method
cpg	213.97	J/mol×K	487.89	Joback Method

cpg	225.00	J/mol×K	524.25	Joback Method
cpg	235.38	J/mol×K	560.62	Joback Method
cpg	245.12	J/mol×K	596.98	Joback Method
cpg	254.26	J/mol×K	633.34	Joback Method
cpg	262.83	J/mol×K	669.70	Joback Method
dvisc	0.0012755	Pa×s	282.57	Joback Method
dvisc	0.0022898	Pa×s	248.78	Joback Method
dvisc	0.0008051	Pa×s	316.36	Joback Method
dvisc	0.0005554	Pa×s	350.15	Joback Method
dvisc	0.0004090	Pa×s	383.95	Joback Method
dvisc	0.0003165	Pa×s	417.74	Joback Method
dvisc	0.0002545	Pa×s	451.53	Joback Method
hvapt	46.40	kJ/mol	402.50	NIST Webbook
hvapt	46.80	kJ/mol	433.00	NIST Webbook
hvapt	46.40	kJ/mol	372.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	359.30	K	4.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41534e+01
Coeff. B	-3.70742e+03
Coeff. C	-6.81820e+01
Temperature range (K), min.	335.56
Temperature range (K), max.	487.48

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=C620166&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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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