Benzene, 1,4-dichloro-2-ethyl-

Other names:	1,4-Dichloro-2-ethylbenzene
	2,5-Dichloro-1,4-dimethylbenzene
	2,5-Dichloroethylbenzene
	Benzene, 1,4-dichloro-3-ethyl
	Benzene, 2,4-dichloro-4-ethyl
	Benzene, 2,5-dichloro-1-ethyl
Inchi:	InChI=1S/C8H8Cl2/c1-2-6-5-7(9)3-4-8(6)10/h3-5H,2H2,1H3
InchiKey:	PZPSDDYNMXBZOA-UHFFFAOYSA-N
Formula:	C8H8Cl2
SMILES:	CCc1cc(Cl)ccc1Cl
Mol. weight [g/mol]:	175.06
CAS:	54484-63-8

Physical Properties

Property code	Value	Unit	Source
gf	85.77	kJ/mol	Joback Method
hf	-26.34	kJ/mol	Joback Method
hfus	18.13	kJ/mol	Joback Method
hvap	45.77	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.556		Crippen Method
mcvol	124.300	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	1213.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1180.00		NIST Webbook
rinpol	1196.00		NIST Webbook
ripol	1658.00		NIST Webbook
ripol	1689.00		NIST Webbook
tb	493.94	K	Joback Method
tc	719.52	K	Joback Method
tf	291.22	K	Joback Method
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.16	J/mol×K	719.52	Joback Method
cpg	273.48	J/mol×K	681.92	Joback Method
cpg	265.25	J/mol×K	644.33	Joback Method
cpg	256.47	J/mol×K	606.73	Joback Method
cpg	247.09	J/mol×K	569.13	Joback Method
cpg	237.10	J/mol×K	531.54	Joback Method
cpg	226.48	J/mol×K	493.94	Joback Method
dvisc	0.0017277	Pa×s	291.22	Joback Method
dvisc	0.0002624	Pa×s	493.94	Joback Method
dvisc	0.0003201	Pa×s	460.15	Joback Method
dvisc	0.0004030	Pa×s	426.37	Joback Method
dvisc	0.0005279	Pa×s	392.58	Joback Method
dvisc	0.0007276	Pa×s	358.79	Joback Method
dvisc	0.0010719	Pa×s	325.01	Joback Method
hvapt	46.00	kJ/mol	400.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37701e+01
Coeff. B	-3.78024e+03
Coeff. C	-7.64390e+01
Temperature range (K), min.	317.62
Temperature range (K), max.	523.35

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=C54484638&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
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