Benzene, 1,3-dichloro-2-ethyl-

Other names: 2,6-Dichloroethylbenzene
Inchi: InChI=1S/C8H8Cl2/c1-2-6-7(9)4-3-5-8(6)10/h3-5H,2H2,1H3
InchiKey: NUDVJQOVBFONPG-UHFFFAOYSA-N
Formula: C8H8Cl2
SMILES: CCc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 175.06
CAS: 33407-02-2

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	1256.00		NIST Webbook
rinpol	1241.00		NIST Webbook
ripol	1718.00		NIST Webbook
ripol	1746.00		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	226.48	J/mol×K	493.94	Joback Method
cpg	237.10	J/mol×K	531.54	Joback Method
cpg	247.09	J/mol×K	569.13	Joback Method
cpg	256.47	J/mol×K	606.73	Joback Method

cpg	265.25	J/mol×K	644.33	Joback Method
cpg	273.48	J/mol×K	681.92	Joback Method
cpg	281.16	J/mol×K	719.52	Joback Method
dvisc	0.0017277	Pa×s	291.22	Joback Method
dvisc	0.0010719	Pa×s	325.01	Joback Method
dvisc	0.0007276	Pa×s	358.79	Joback Method
dvisc	0.0005279	Pa×s	392.58	Joback Method
dvisc	0.0004030	Pa×s	426.37	Joback Method
dvisc	0.0003201	Pa×s	460.15	Joback Method
dvisc	0.0002624	Pa×s	493.94	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C33407022&Units=SI

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical 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