Benzene, 1,2,3-trichloro-4-ethyl

Other names: 2,3,4-Trichloro ethylbenzene
Inchi: InChI=1S/C8H7Cl3/c1-2-5-3-4-6(9)8(11)7(5)10/h3-4H,2H2,1H3
InchiKey: JRNXNDCCMJUMKK-UHFFFAOYSA-N
Formula: C8H7Cl3
SMILES: CCc1ccc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 209.50

Physical Properties

Property code	Value	Unit	Source
gf	64.21	kJ/mol	Joback Method
hf	-53.55	kJ/mol	Joback Method
hfus	21.94	kJ/mol	Joback Method
hvap	50.82	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.209		Crippen Method
mcvol	136.540	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1423.00		NIST Webbook
rinpol	1403.00		NIST Webbook
ripol	1940.00		NIST Webbook
ripol	1973.00		NIST Webbook
tb	536.35	K	Joback Method
tc	768.20	K	Joback Method
tf	333.66	K	Joback Method
vc	0.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.30	J/mol×K	536.35	Joback Method
cpg	257.88	J/mol×K	574.99	Joback Method
cpg	266.86	J/mol×K	613.63	Joback Method
cpg	275.28	J/mol×K	652.27	Joback Method
cpg	283.16	J/mol×K	690.91	Joback Method

cpg	290.52	J/mol×K	729.55	Joback Method
cpg	297.38	J/mol×K	768.20	Joback Method
dvisc	0.0013528	Pa×s	333.66	Joback Method
dvisc	0.0009054	Pa×s	367.44	Joback Method
dvisc	0.0006484	Pa×s	401.22	Joback Method
dvisc	0.0004890	Pa×s	435.00	Joback Method
dvisc	0.0003841	Pa×s	468.79	Joback Method
dvisc	0.0003117	Pa×s	502.57	Joback Method
dvisc	0.0002597	Pa×s	536.35	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=R13325&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

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