2,4,5-Trichloro ethylbenzene

Other names: Benzene, 1,2,4-trichloro-5-ethyl
Inchi: InChI=1S/C8H7Cl3/c1-2-5-3-7(10)8(11)4-6(5)9/h3-4H,2H2,1H3
InchiKey: GEHSSDLJJSJBLT-UHFFFAOYSA-N
Formula: C8H7Cl3
SMILES: CCc1cc(Cl)c(Cl)cc1Cl
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	1349.00		NIST Webbook
rinpol	1366.00		NIST Webbook
ripol	1863.00		NIST Webbook
ripol	1890.00		NIST Webbook
ripol	1863.00		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	290.52	J/mol×K	729.55	Joback Method
cpg	283.16	J/mol×K	690.91	Joback Method
cpg	275.28	J/mol×K	652.27	Joback Method

cpg	266.86	J/mol×K	613.63	Joback Method
cpg	257.88	J/mol×K	574.99	Joback Method
cpg	297.38	J/mol×K	768.20	Joback Method
dvisc	0.0002597	Pa×s	536.35	Joback Method
dvisc	0.0003117	Pa×s	502.57	Joback Method
dvisc	0.0003841	Pa×s	468.79	Joback Method
dvisc	0.0004890	Pa×s	435.00	Joback Method
dvisc	0.0006484	Pa×s	401.22	Joback Method
dvisc	0.0009054	Pa×s	367.44	Joback Method
dvisc	0.0013528	Pa×s	333.66	Joback Method

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=R13343&Units=SI
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
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