1',1',2',2-Tetrachloro ethyl benzene

Inchi: InChI=1S/C8H6Cl4/c9-5-8(11,12)6-3-1-2-4-7(6)10/h1-4H,5H2
InchiKey: IBKZXJDBUSOMOE-UHFFFAOYSA-N
Formula: C8H6Cl4
SMILES: ClCC(Cl)(Cl)c1ccccc1Cl
Mol. weight [g/mol]: 243.94
CAS: 116401-13-9

Physical Properties

Property code	Value	Unit	Source
gf	74.38	kJ/mol	Joback Method
hf	-55.10	kJ/mol	Joback Method
hfus	19.50	kJ/mol	Joback Method
hvap	52.58	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	4.209		Crippen Method
mcvol	148.780	ml/mol	McGowan Method
pc	3089.85	kPa	Joback Method
tb	560.59	K	Joback Method
tc	810.28	K	Joback Method
tf	340.96	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.72	J/mol×K	560.59	Joback Method
cpg	285.80	J/mol×K	602.21	Joback Method
cpg	294.92	J/mol×K	643.82	Joback Method
cpg	303.14	J/mol×K	685.44	Joback Method
cpg	310.55	J/mol×K	727.05	Joback Method
cpg	317.24	J/mol×K	768.67	Joback Method
cpg	323.29	J/mol×K	810.28	Joback Method
dvisc	0.0023479	Pa×s	340.96	Joback Method
dvisc	0.0013403	Pa×s	377.56	Joback Method

dvisc	0.0008448	Pa×s	414.17	Joback Method
dvisc	0.0005739	Pa×s	450.77	Joback Method
dvisc	0.0004132	Pa×s	487.38	Joback Method
dvisc	0.0003115	Pa×s	523.98	Joback Method
dvisc	0.0002436	Pa×s	560.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401139&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume