Benzene, (1,3,3,3-tetrachloropropyl)-

Other names: (1,3,3,3-tetrachloropropyl)benzene
Inchi: InChI=1S/C9H8Cl4/c10-8(6-9(11,12)13)7-4-2-1-3-5-7/h1-5,8H,6H2
InchiKey: JJRCOEWDFJHOFK-UHFFFAOYSA-N
Formula: C9H8Cl4
SMILES: ClC(CC(Cl)(Cl)Cl)c1ccccc1
Mol. weight [g/mol]: 257.97
CAS: 23691-27-2

Physical Properties

Property code	Value	Unit	Source
gf	89.99	kJ/mol	Joback Method
hf	-69.55	kJ/mol	Joback Method
hfus	18.96	kJ/mol	Joback Method
hvap	53.76	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.727		Crippen Method
mcvol	162.870	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
rinpol	1547.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1547.00		NIST Webbook
tb	578.05	K	Joback Method
tc	826.94	K	Joback Method
tf	324.71	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.27	J/mol×K	578.05	Joback Method
cpg	369.54	J/mol×K	785.46	Joback Method
cpg	361.76	J/mol×K	743.98	Joback Method
cpg	353.13	J/mol×K	702.50	Joback Method
cpg	343.58	J/mol×K	661.01	Joback Method

cpg	332.99	J/mol×K	619.53	Joback Method
cpg	376.59	J/mol×K	826.94	Joback Method
dvisc	0.0002075	Pa×s	578.05	Joback Method
dvisc	0.0002784	Pa×s	535.83	Joback Method
dvisc	0.0003927	Pa×s	493.60	Joback Method
dvisc	0.0005908	Pa×s	451.38	Joback Method
dvisc	0.0009670	Pa×s	409.16	Joback Method
dvisc	0.0017726	Pa×s	366.93	Joback Method
dvisc	0.0038043	Pa×s	324.71	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=C23691272&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume