Benzene, (3,3,3-trichloro-1-methylenepropyl)

Inchi: InChI=1S/C10H9Cl3/c1-8(7-10(11,12)13)9-5-3-2-4-6-9/h2-6H,1,7H2
InchiKey: JNHUFDXYWPRKLK-UHFFFAOYSA-N
Formula: C10H9Cl3
SMILES: C=C(CC(Cl)(Cl)Cl)c1ccccc1
Mol. weight [g/mol]: 235.54

Physical Properties

Property code	Value	Unit	Source
gf	192.07	kJ/mol	Joback Method
hf	46.47	kJ/mol	Joback Method
hfus	18.28	kJ/mol	Joback Method
hvap	51.40	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.460		Crippen Method
mcvol	160.420	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1495.00		NIST Webbook
rinpol	1495.00		NIST Webbook
tb	560.50	K	Joback Method
tc	804.94	K	Joback Method
tf	305.34	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.40	J/mol×K	560.50	Joback Method
cpg	335.23	J/mol×K	601.24	Joback Method
cpg	346.88	J/mol×K	641.98	Joback Method
cpg	357.45	J/mol×K	682.72	Joback Method
cpg	367.05	J/mol×K	723.46	Joback Method
cpg	375.77	J/mol×K	764.20	Joback Method
cpg	383.71	J/mol×K	804.94	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=R514926&Units=SI

Legend

cpg:	Ideal gas heat capacity
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

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