Benzene, (2,2,2-trichloroethyl)-

Inchi: InChI=1S/C8H7Cl3/c9-8(10,11)6-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey: XFEKIQFBJSDMQB-UHFFFAOYSA-N
Formula: C8H7Cl3
SMILES: ClC(Cl)(Cl)Cc1ccccc1
Mol. weight [g/mol]: 209.50
CAS: 3883-13-4

Physical Properties

Property code	Value	Unit	Source
gf	95.94	kJ/mol	Joback Method
hf	-27.89	kJ/mol	Joback Method
hfus	15.69	kJ/mol	Joback Method
hvap	47.54	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.599		Crippen Method
mcvol	136.540	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
rinpol	1301.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1301.00		NIST Webbook
tb	518.18	K	Joback Method
tc	762.22	K	Joback Method
tf	298.52	K	Joback Method
vc	0.511	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.16	J/mol×K	518.18	Joback Method
cpg	302.14	J/mol×K	721.54	Joback Method
cpg	294.36	J/mol×K	680.87	Joback Method
cpg	285.76	J/mol×K	640.20	Joback Method
cpg	276.25	J/mol×K	599.53	Joback Method
cpg	265.75	J/mol×K	558.85	Joback Method

cpg	309.17	J/mol×K	762.22	Joback Method
dvisc	0.0002703	Pa×s	518.18	Joback Method
dvisc	0.0003547	Pa×s	481.57	Joback Method
dvisc	0.0004867	Pa×s	444.96	Joback Method
dvisc	0.0007068	Pa×s	408.35	Joback Method
dvisc	0.0011046	Pa×s	371.74	Joback Method
dvisc	0.0019034	Pa×s	335.13	Joback Method
dvisc	0.0037480	Pa×s	298.52	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=C3883134&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

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