Benzene, (2,2-dichloro-1-methylcyclopropyl)-

Other names:	(2,2-Dichloro-1-methylcyclopropyl)benzene
Inchi:	InChI=1S/C10H10Cl2/c1-9(7-10(9,11)12)8-5-3-2-4-6-8/h2-6H,7H2,1H3
InchiKey:	NXYPRVQXSWVEOB-UHFFFAOYSA-N
Formula:	C10H10Cl2
SMILES:	CC1(c2ccccc2)CC1(Cl)Cl
Mol. weight [g/mol]:	201.09
CAS:	3591-42-2

Physical Properties

Property code	Value	Unit	Source
gf	163.93	kJ/mol	Joback Method
hf	38.26	kJ/mol	Joback Method
hfus	10.70	kJ/mol	Joback Method
hvap	46.20	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.522		Crippen Method
mcvol	141.620	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
tb	532.29	K	Joback Method
tc	786.07	K	Joback Method
tf	350.22	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.45	J/mol×K	532.29	Joback Method
cpg	312.50	J/mol×K	574.59	Joback Method
cpg	325.07	J/mol×K	616.88	Joback Method
cpg	336.55	J/mol×K	659.18	Joback Method
cpg	347.29	J/mol×K	701.48	Joback Method
cpg	357.68	J/mol×K	743.77	Joback Method
cpg	368.09	J/mol×K	786.07	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	349.20	K	0.10	NIST Webbook

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=C3591422&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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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