

trans-1,2-Dimethyl-3,3-dichlorocyclopropane

Inchi:	InChI=1S/C5H8Cl2/c1-3-4(2)5(3,6)7/h3-4H,1-2H3/t3-,4-/m0/s1
InchiKey:	KOBPHDGNTMLQKI-IMJSIDKUSA-N
Formula:	C5H8Cl2
SMILES:	CC1C(C)C1(Cl)Cl
Mol. weight [g/mol]:	139.02
CAS:	1120-68-9

Physical Properties

Property code	Value	Unit	Source
chl	-3067.90 ± 1.10	kJ/mol	NIST Webbook
gf	7.20	kJ/mol	Joback Method
hf	-130.65	kJ/mol	Joback Method
hfl	-90.00 ± 1.00	kJ/mol	NIST Webbook
hfus	11.08	kJ/mol	Joback Method
hvap	33.64	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	2.446		Crippen Method
mcvol	94.930	ml/mol	McGowan Method
pc	3615.89	kPa	Joback Method
tb	386.30	K	Joback Method
tc	591.56	K	Joback Method
tf	239.31	K	Joback Method
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	161.12	J/molxK	386.30	Joback Method
cpg	172.41	J/molxK	420.51	Joback Method
cpg	182.72	J/molxK	454.72	Joback Method
cpg	192.16	J/molxK	488.93	Joback Method
cpg	200.81	J/molxK	523.14	Joback Method
cpg	208.78	J/molxK	557.35	Joback Method
cpg	216.17	J/molxK	591.56	Joback Method

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=C1120689&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

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