

1-Propene, 1,1-dichloro-2-methyl-

Inchi:	InChI=1S/C4H6Cl2/c1-3(2)4(5)6/h1-2H3
InchiKey:	GSQMUEGXIDQJES-UHFFFAOYSA-N
Formula:	C4H6Cl2
SMILES:	CC(C)=C(Cl)Cl
Mol. weight [g/mol]:	125.00
CAS:	6065-93-6

Physical Properties

Property code	Value	Unit	Source
gf	22.06	kJ/mol	Joback Method
hf	-59.73	kJ/mol	Joback Method
hfus	12.09	kJ/mol	Joback Method
hvap	33.39	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.715		Crippen Method
mcvol	87.400	ml/mol	McGowan Method
pc	3838.78	kPa	Joback Method
rinpol	748.00		NIST Webbook
rinpol	748.00		NIST Webbook
tb	369.70	K	Joback Method
tc	569.83	K	Joback Method
tf	161.68	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	126.90	J/mol×K	369.70	Joback Method
cpg	134.07	J/mol×K	403.06	Joback Method
cpg	140.80	J/mol×K	436.41	Joback Method
cpg	147.12	J/mol×K	469.77	Joback Method
cpg	153.05	J/mol×K	503.12	Joback Method
cpg	158.62	J/mol×K	536.48	Joback Method
cpg	163.85	J/mol×K	569.83	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=C6065936&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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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