

1-Propene, 3-chloro-2-(chloromethyl)-

Other names:	1,3-Dichloro-2-methylenepropane Propene, 3-chloro-2-(chloromethyl)- 2-Chloromethyl-3-chloropropene 2-Methylene-1,3-dichloropropane 2-Methylenepropane-1,3-dichloride 3-Chloro-2-(chloromethyl)propene 3-Chloro-2-chloromethyl-1-propene
Inchi:	InChI=1S/C4H6Cl2/c1-4(2-5)3-6/h1-3H2
InchiKey:	XJFZOSUFGSANIF-UHFFFAOYSA-N
Formula:	C4H6Cl2
SMILES:	C=C(CCl)CCl
Mol. weight [g/mol]:	125.00
CAS:	1871-57-4

Physical Properties

Property code	Value	Unit	Source
gf	38.23	kJ/mol	Joback Method
hf	-41.73	kJ/mol	Joback Method
hfus	11.92	kJ/mol	Joback Method
hvap	32.68	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	2.020		Crippen Method
mcvol	87.400	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	799.00		NIST Webbook
rinpol	799.00		NIST Webbook
tb	411.20	K	NIST Webbook
tc	552.14	K	Joback Method
tf	178.96	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	128.45	J/mol×K	362.34	Joback Method
cpg	135.17	J/mol×K	393.97	Joback Method
cpg	141.55	J/mol×K	425.61	Joback Method
cpg	147.59	J/mol×K	457.24	Joback Method
cpg	153.31	J/mol×K	488.87	Joback Method
cpg	158.73	J/mol×K	520.51	Joback Method
cpg	163.86	J/mol×K	552.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1871574&Units=SI
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

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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