1-Propene, 1,3-dichloro-2-chloromethyl

Inchi: InChI=1S/C4H5Cl3/c5-1-4(2-6)3-7/h1H,2-3H2
InchiKey: HPBWGILCMWDPPJ-UHFFFAOYSA-N
Formula: C4H5Cl3
SMILES: ClC=C(CCl)CCl
Mol. weight [g/mol]: 159.44

Physical Properties

Property code	Value	Unit	Source
gf	18.68	kJ/mol	Joback Method
hf	-65.68	kJ/mol	Joback Method
hfus	17.60	kJ/mol	Joback Method
hvap	37.69	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.587		Crippen Method
mcvol	99.640	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	969.00		NIST Webbook
rinpol	969.00		NIST Webbook
tb	407.25	K	Joback Method
tc	611.67	K	Joback Method
tf	205.56	K	Joback Method
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.80	J/mol×K	407.25	Joback Method
cpg	154.46	J/mol×K	441.32	Joback Method
cpg	160.68	J/mol×K	475.39	Joback Method
cpg	166.47	J/mol×K	509.46	Joback Method
cpg	171.87	J/mol×K	543.53	Joback Method
cpg	176.91	J/mol×K	577.60	Joback Method
cpg	181.61	J/mol×K	611.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R12391&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

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