1-Butene, 2-(chloromethyl)-

Other names: «beta»-Ethallyl chloride
Inchi: InChI=1S/C5H9Cl/c1-3-5(2)4-6/h2-4H2,1H3
InchiKey: LTVNYBFQRYQEJU-UHFFFAOYSA-N
Formula: C5H9Cl
SMILES: C=C(CC)CCl
Mol. weight [g/mol]: 104.58
CAS: 23010-02-8

Physical Properties

Property code	Value	Unit	Source
gf	58.58	kJ/mol	Joback Method
hf	-46.63	kJ/mol	Joback Method
hfus	10.31	kJ/mol	Joback Method
hvap	30.52	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	2.191		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
pc	3509.58	kPa	Joback Method
rinpol	696.00		NIST Webbook
rinpol	694.00		NIST Webbook
tb	347.79	K	Joback Method
tc	527.66	K	Joback Method
tf	160.31	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.14	J/mol×K	347.79	Joback Method
cpg	146.61	J/mol×K	377.77	Joback Method
cpg	154.71	J/mol×K	407.75	Joback Method
cpg	162.44	J/mol×K	437.72	Joback Method
cpg	169.84	J/mol×K	467.70	Joback Method
cpg	176.89	J/mol×K	497.68	Joback Method

cpg	183.63	J/mol×K	527.66	Joback Method

Sources

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=C23010028&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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