1,3-Butadiene, 2-(chloromethyl)

Inchi: InChI=1S/C5H7Cl/c1-3-5(2)4-6/h3H,1-2,4H2
InchiKey: WOZCYBXTBXAJSA-UHFFFAOYSA-N
Formula: C5H7Cl
SMILES: C=CC(=C)CCl
Mol. weight [g/mol]: 102.56

Physical Properties

Property code	Value	Unit	Source
gf	146.42	kJ/mol	Joback Method
hf	78.80	kJ/mol	Joback Method
hfus	9.03	kJ/mol	Joback Method
hvap	29.85	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.967		Crippen Method
mcvol	84.950	ml/mol	McGowan Method
pc	3690.97	kPa	Joback Method
rinpol	730.00		NIST Webbook
tb	344.47	K	Joback Method
tc	528.29	K	Joback Method
tf	158.55	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.28	J/mol×K	344.47	Joback Method
cpg	133.07	J/mol×K	375.11	Joback Method
cpg	140.45	J/mol×K	405.74	Joback Method
cpg	147.46	J/mol×K	436.38	Joback Method
cpg	154.11	J/mol×K	467.01	Joback Method
cpg	160.40	J/mol×K	497.65	Joback Method
cpg	166.37	J/mol×K	528.29	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R510855&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