trans-1-Chloro-3-methyl-1-butene

Inchi: InChI=1S/C5H9Cl/c1-5(2)3-4-6/h3-5H,1-2H3/b4-3+
InchiKey: MXVSJNLRVLKAOG-ONEGZZNKSA-N
Formula: C5H9Cl
SMILES: CC(C)C=CCl
Mol. weight [g/mol]: 104.58
CAS: 66213-68-1

Physical Properties

Property code	Value	Unit	Source
gf	57.07	kJ/mol	Joback Method
hf	-50.33	kJ/mol	Joback Method
hfus	9.58	kJ/mol	Joback Method
hvap	30.68	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	2.395		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
pc	3564.27	kPa	Joback Method
tb	354.95	K	Joback Method
tc	541.48	K	Joback Method
tf	155.95	K	Joback Method
vc	0.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.80	J/mol×K	354.95	Joback Method
cpg	145.84	J/mol×K	386.04	Joback Method
cpg	154.44	J/mol×K	417.13	Joback Method
cpg	162.59	J/mol×K	448.21	Joback Method
cpg	170.33	J/mol×K	479.30	Joback Method
cpg	177.68	J/mol×K	510.39	Joback Method
cpg	184.64	J/mol×K	541.48	Joback Method
dvisc	0.0074259	Pa×s	155.95	Joback Method
dvisc	0.0025041	Pa×s	189.12	Joback Method

dvisc	0.0011680	Pa×s	222.28	Joback Method
dvisc	0.0006641	Pa×s	255.45	Joback Method
dvisc	0.0004299	Pa×s	288.62	Joback Method
dvisc	0.0003044	Pa×s	321.78	Joback Method
dvisc	0.0002299	Pa×s	354.95	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39273e+01
Coeff. B	-3.10959e+03
Coeff. C	-4.29400e+01
Temperature range (K), min.	270.92
Temperature range (K), max.	403.85

Sources

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=C66213681&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume