Trans-1-chloro-1-butene

Inchi: InChI=1S/C4H7Cl/c1-2-3-4-5/h3-4H,2H2,1H3/b4-3+
InchiKey: DUDKKPVINWLFBI-ONEGZZNKSA-N
Formula: C4H7Cl
SMILES: CCC=CCl
Mol. weight [g/mol]: 90.55
CAS: 7611-87-2

Physical Properties

Property code	Value	Unit	Source
gf	51.09	kJ/mol	Joback Method
hf	-16.50	kJ/mol	NIST Webbook
hfus	10.51	kJ/mol	Joback Method
hvap	28.84	kJ/mol	Joback Method
log10ws	-2.00		Crippen Method
logp	2.149		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
pc	3970.51	kPa	Joback Method
tb	341.25 ± 1.00	K	NIST Webbook
tb	341.25 ± 1.00	K	NIST Webbook
tb	341.20	K	NIST Webbook
tc	514.66	K	Joback Method
tf	159.68	K	Joback Method
vc	0.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	104.96	J/mol×K	332.51	Joback Method
cpg	112.16	J/mol×K	362.87	Joback Method
cpg	118.99	J/mol×K	393.23	Joback Method
cpg	125.48	J/mol×K	423.59	Joback Method
cpg	131.63	J/mol×K	453.95	Joback Method
cpg	137.47	J/mol×K	484.30	Joback Method
cpg	143.01	J/mol×K	514.66	Joback Method

dvisc	0.0033962	Pa×s	159.68	Joback Method
dvisc	0.0015278	Pa×s	188.49	Joback Method
dvisc	0.0008494	Pa×s	217.29	Joback Method
dvisc	0.0005418	Pa×s	246.09	Joback Method
dvisc	0.0003798	Pa×s	274.90	Joback Method
dvisc	0.0002848	Pa×s	303.70	Joback Method
dvisc	0.0002244	Pa×s	332.51	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.33670e+01
Coeff. B	-2.26234e+03
Coeff. C	-8.26080e+01
Temperature range (K), min.	255.58
Temperature range (K), max.	363.52

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7611872&Units=SI

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

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