Trans-1-chloro-1,3-butadiene

Inchi: InChI=1S/C4H5Cl/c1-2-3-4-5/h2-4H,1H2/b4-3+
InchiKey: PCPYTNCQOSFKGG-ONEGZZNKSA-N
Formula: C4H5Cl
SMILES: C=CC=CCl
Mol. weight [g/mol]: 88.54
CAS: 16503-25-6

Physical Properties

Property code	Value	Unit	Source
gf	138.93	kJ/mol	Joback Method
hf	101.02	kJ/mol	Joback Method
hfus	9.23	kJ/mol	Joback Method
hvap	28.17	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.925		Crippen Method
mcvol	70.860	ml/mol	McGowan Method
pc	4189.32	kPa	Joback Method
tb	329.19	K	Joback Method
tc	515.39	K	Joback Method
tf	157.92	K	Joback Method
vc	0.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	92.71	J/mol×K	329.19	Joback Method
cpg	99.18	J/mol×K	360.22	Joback Method
cpg	105.27	J/mol×K	391.26	Joback Method
cpg	110.99	J/mol×K	422.29	Joback Method
cpg	116.36	J/mol×K	453.32	Joback Method
cpg	121.40	J/mol×K	484.36	Joback Method
cpg	126.13	J/mol×K	515.39	Joback Method
dvisc	0.0026718	Pa×s	157.92	Joback Method
dvisc	0.0012672	Pa×s	186.47	Joback Method

dvisc	0.0007327	Pa×s	215.01	Joback Method
dvisc	0.0004817	Pa×s	243.56	Joback Method
dvisc	0.0003458	Pa×s	272.10	Joback Method
dvisc	0.0002644	Pa×s	300.64	Joback Method
dvisc	0.0002118	Pa×s	329.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16503256&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume