3-Chloro-3-methyl-1-butene

Inchi: InChI=1S/C5H9Cl/c1-4-5(2,3)6/h4H,1H2,2-3H3
InchiKey: KECJPTAJLDCQHM-UHFFFAOYSA-N
Formula: C5H9Cl
SMILES: C=CC(C)(C)Cl
Mol. weight [g/mol]: 104.58
CAS: 2190-48-9

Physical Properties

Property code	Value	Unit	Source
af	0.1768		Cheméo Relay (1.0)
gf	69.97	kJ/mol	Joback Method
hf	-97.68	kJ/mol	Cheméo Relay (1.0)
hfus	4.21	kJ/mol	Joback Method
hvap	30.81	kJ/mol	Cheméo Relay (1.0)
ie	9.92	eV	Cheméo Relay (1.0)
log10ws	-2.21		Cheméo Relay (1.0)
logp	2.190		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
rinpol	642.00		NIST Webbook
rinpol	642.00		NIST Webbook
tb	340.20	K	Cheméo Relay (1.0)
tc	537.54	K	Cheméo Relay (1.0)
tf	190.60	K	Cheméo Relay (1.0)
vc	0.325	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.59	J/mol×K	344.68	Joback Method
cpg	189.65	J/mol×K	533.30	Joback Method
cpg	182.43	J/mol×K	501.86	Joback Method
cpg	174.73	J/mol×K	470.42	Joback Method
cpg	166.52	J/mol×K	438.99	Joback Method

cpg	157.78	J/mol×K	407.55	Joback Method
cpg	148.48	J/mol×K	376.12	Joback Method
dvisc	0.0009575	Pa×s	260.69	Joback Method
dvisc	0.0003336	Pa×s	344.68	Joback Method
dvisc	0.0004455	Pa×s	316.68	Joback Method
dvisc	0.0006293	Pa×s	288.68	Joback Method
dvisc	0.0074890	Pa×s	176.69	Joback Method
dvisc	0.0016115	Pa×s	232.69	Joback Method
dvisc	0.0031275	Pa×s	204.69	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.28437e+01
Coeff. B	-2.77734e+03
Coeff. C	-3.93260e+01
Temperature range (K), min.	260.52
Temperature range (K), max.	408.05

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2190489&Units=SI

Legend

af: Acentric Factor

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume