Propane, 1,3-dichloro-2-methyl-

Other names: 1,3-Dichloro-2-methylpropane
1,3-Dichloroisobutane
Inchi: InChI=1S/C4H8Cl2/c1-4(2-5)3-6/h4H,2-3H2,1H3
InchiKey: VENSUTAUIFXSRD-UHFFFAOYSA-N
Formula: C4H8Cl2
SMILES: CC(CCl)CCl
Mol. weight [g/mol]: 127.01
CAS: 616-19-3

Physical Properties

Property code	Value	Unit	Source
gf	-43.50	kJ/mol	Joback Method
hf	-162.65	kJ/mol	Joback Method
hfus	10.99	kJ/mol	Joback Method
hvap	32.88	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	2.100		Crippen Method
mcvol	91.700	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	820.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	820.00		NIST Webbook
tb	365.34	K	Joback Method
tc	551.71	K	Joback Method
tf	179.68	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.54	J/mol×K	551.71	Joback Method
cpg	141.59	J/mol×K	365.34	Joback Method
cpg	149.22	J/mol×K	396.40	Joback Method
cpg	156.51	J/mol×K	427.46	Joback Method

cpg	163.48	J/mol×K	458.52	Joback Method
cpg	170.14	J/mol×K	489.58	Joback Method
cpg	176.48	J/mol×K	520.65	Joback Method
dvisc	0.0003376	Pa×s	365.34	Joback Method
dvisc	0.0069129	Pa×s	179.68	Joback Method
dvisc	0.0028879	Pa×s	210.62	Joback Method
dvisc	0.0015088	Pa×s	241.57	Joback Method
dvisc	0.0009135	Pa×s	272.51	Joback Method
dvisc	0.0006126	Pa×s	303.45	Joback Method
dvisc	0.0004424	Pa×s	334.40	Joback Method
hvapt	45.10	kJ/mol	339.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	318.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47516e+01
Coeff. B	-3.00016e+03
Coeff. C	-9.93590e+01
Temperature range (K), min.	306.78
Temperature range (K), max.	417.17

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C616193&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

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
hvapt:	Enthalpy of vaporization at a given temperature
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume